

Isogeometric sensitivity-enhanced polynomial chaos expansion under geometric uncertainty

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Abstract

Geometric uncertainty remains a significant challenge in engineering applications, as shape variations can substantially affect mechanical response and make response-only polynomial chaos expansion (PCE) surrogates sample-demanding. Accordingly, this paper proposes an isogeometric sensitivity-enhanced PCE for systems characterized by a small set of uncertain geometric parameters. The key idea is to enrich the surrogate with geometry-consistent derivatives obtained from the same isogeometric analysis (IGA) model used to solve the mechanical problem. Within this framework, geometry, mechanical analysis, and variational sensitivity evaluation share a common NURBS-based representation. The approach is assessed through two- and three-dimensional linear elasticity benchmarks, a nonlinear Neo-Hookean problem, and a case combining geometric and material uncertainty. Across these examples, sensitivity enrichment generally improves global response and gradient prediction relative to response-only sparse PCE, with the clearest gains observed in low- and intermediate-data regimes. Cost-aware comparisons with gradient-enhanced Kriging show competitive accuracy while avoiding the additional high-fidelity response evaluations required for finite-difference gradients. Overall, the results indicate that IGA-derived variational sensitivities can improve the data efficiency of PCE-based uncertainty quantification under low-dimensional geometric variability, with gains varying across benchmarks and metrics. *Keywords:* Polynomial Chaos Expansion (PCE), Isogeometric Analysis (IGA), Geometric Uncertainty, Variational Sensitivity Analysis, Gradient-enhanced Surrogate Modeling, Constrained Regression

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Highlights

- Develops a sensitivity-enhanced polynomial chaos expansion for geometric uncertainty.
- Uses isogeometric analysis to preserve geometry and avoid remeshing.
- Derives variational sensitivities for linear and nonlinear Neo-Hookean mechanics.
- Improves low-data response and gradient accuracy under geometric uncertainty.
- Benchmarks cost–accuracy against finite-difference gradient-enhanced Kriging.

1. Introduction

Geometric uncertainties arise in a wide range of engineering applications, from aerospace structures to biomedical devices, where performance and reliability are closely tied to geometric precision [1, 2, 3]. The origins of these geometric variations can be attributed to manufacturing processes, construction technologies and methods, environmental conditions, and long-term service requirements [4]. Even small deviations in thickness, curvature, length, or overall shape may alter load paths, trigger stress concentrations, or shift natural frequencies [5, 6]. When uncertainty is represented through geometric parameterizations, the variability modifies the spatial domain on which the governing partial differential equations (PDEs) are posed. As a result, geometric variations affect the numerical model through the domain geometry, the integration mappings, and the resulting mathematical operators characterizing the physics of the problem. For uncertainty quantification (UQ), the main difficulty is to characterize these geometry-dependent responses across the uncertain parameter space when only a limited number of high-fidelity model evaluations is affordable.

Recent studies have investigated how geometric and fabrication-induced variability influence structural response, highlighting the practical relevance of geometry-driven uncertainty in mechanical systems [7, 8, 9]. Nevertheless, in many numerical workflows, geometry is still approximated through conventional finite element discretizations, and repeated analyses over different geometric realizations may require remeshing or repeated model updates. These issues can increase the computational burden and may introduce inconsistencies between the geometric parameterization, the mechanical analysis, and the derivative information used for surrogate construction.

This work focuses on geometric uncertainties described by a small number of independent random variables controlling global shape parameters. Such low-dimensional parametric descriptions are relevant in design studies and controlled uncertainty propagation settings, where dominant geometric features such as radii, thicknesses, lengths, or characteristic dimensions are uncertain. Within this scope, an effective UQ strategy should satisfy two requirements: it should represent the geometry consistently as the uncertain parameters vary, and it should propagate the resulting variability efficiently through the mechanical model. The present paper addresses these two aspects by combining Isogeometric Analysis (IGA) with a sensitivity-enhanced PCE formulation.

IGA contributes to geometric consistency by unifying design and analysis within a common geometric representation [10, 11]. By employing Computer-Aided Design (CAD) descriptions, commonly represented by Non-Uniform Rational B-Splines (NURBS), directly in the analysis, IGA can reduce or avoid the geometric approximation introduced by conventional mesh-based discretizations. When the geometry is exactly represented by the underlying spline basis, its description is preserved independently of the refinement level used for the analysis. This makes IGA a natural framework for problems in which uncertainty acts primarily through changes in shape [12, 13]. It provides a consistent setting in which geometry definition, numerical analysis, and variational sensitivity evaluation [14, 15] are formulated using the same basis functions and geometric parameterization. This consistency is particularly relevant when derivative information with respect to geometric parameters is incorporated into a surrogate model, since the resulting sensitivities remain directly tied to the same parameterization used in the mechanical analysis. Although the numerical examples considered here are deliberately simple proof-of-concept cases, this geometry–analysis–sensitivity consistency provides a useful basis for extending the framework to more complex CAD-based configurations. IGA formulations have also been extended to geometrically nonlinear structural analyses, including laminated composite plates and shells [16], and incremental or continuation-based strategies have demonstrated the capability of NURBS-based discretizations to capture large deformation and path-dependent responses [17].

The second aspect concerns the efficient propagation of uncertainty once the geometry-dependent mechanical model has been defined. PCE represents the stochastic response as a series of orthogonal polynomials of the underlying random variables or stochastic germs [18, 19, 20]. Sparse regression approaches, including least-angle regression (LAR), make PCE suitable when only a limited number of training samples is available [21]. Compared with purely sampling-based es-

timators, PCE exploits a structured spectral representation of the stochastic response and can achieve rapid convergence for sufficiently smooth quantities of interest [22]. Polynomial chaos expansions have also been leveraged as analytical tools for estimating fractional moments and reconstructing response distributions, providing stable alternatives when simulations are costly [23]. Nevertheless, when uncertainty acts through geometric parameterizations, response-only PCE constructions may remain sample-demanding. Improving sample efficiency therefore motivates the use of additional information beyond response evaluations alone.

A natural strategy for enriching surrogate construction is to incorporate derivative information. Gradient-enhanced surrogate modeling has been explored across response surface approximations, weighted least-squares formulations, gradient-enhanced Kriging, co-Kriging, radial basis functions, and support vector regression [24, 25, 26]. These methods show that derivative information can improve local fidelity and reduce the number of samples required to construct accurate approximations when gradients are available at moderate additional cost. For geometry-driven uncertainty, however, an additional requirement arises: the derivative information should be consistent with the geometric parameterization defining the mechanical model. This motivates the use of IGA-derived variational sensitivities, which provide mechanically meaningful derivatives of the response with respect to the uncertain geometric parameters.

Within the PCE family, constrained regression provides another route for incorporating additional information into the surrogate construction. Physics-informed PCE (PC^2) extends the polynomial chaos expansion framework by embedding governing-equation information directly into the coefficient estimation [27, 28]. Physics-informed formulations have gained increasing attention for enhancing model consistency and robustness in data-scarce regimes [29]. In operator-based PC^2 , a Lagrange-multiplier formulation leads to a Karush–Kuhn–Tucker (KKT) system that combines data fidelity with constraints associated with the governing equations or boundary conditions [30]. The present work adopts the same constrained-regression perspective, but does not enforce PDE residuals or boundary conditions through differential operators acting on the polynomial basis. Instead, the constrained-regression structure is used to incorporate variational sensitivities computed from the underlying IGA model. The underlying Moore–Penrose KKT-based construction is retained, while the source of constraint information is changed from operator-based residuals to geometry-consistent sensitivity information. For this reason, the proposed method is better understood as an IGA-based sensitivity-enhanced PCE formulation for geometric uncertainty

120 quantification.

121 Several approaches have been developed to propagate geometric uncertainty. Early PCE-based
122 methods relied on mesh-node parameterizations combined with repeated finite element remesh-
123 ing [31]. Other formulations introduced geometric variability indirectly through thresholding
124 strategies or random-field perturbations of material distributions, where the domain is inferred
125 through a stochastic projection field rather than parameterized explicitly [32]. Stochastic-domain
126 approaches improved efficiency through fictitious domains [33] and mapping techniques [34]. Build-
127 ing on spline-based geometric representations, Stochastic Isogeometric Analysis (SIGA) leveraged
128 NURBS basis functions to represent shape variability more consistently [35]. More recent spec-
129 tral approaches, such as derivative-based sparse Poincaré chaos expansions, have incorporated
130 solver-gradient information into regression-based polynomial surrogate constructions for global
131 sensitivity analysis and Sobol’ index estimation [36]. In the present work, derivative informa-
132 tion is instead obtained from geometry-consistent variational sensitivities within the IGA model
133 and incorporated into the PCE regression for geometric uncertainty quantification. In parallel,
134 nonintrusive PCE frameworks have been applied to systems with geometric deviations [37], often
135 treating geometry through a small number of scalar parameters and relying on repeated high-
136 fidelity simulations, such as computational fluid dynamics (CFD) evaluations, for each stochastic
137 realization. These contributions have significantly advanced the treatment of geometric variability.
138 However, the combined use of CAD-consistent geometric parameterization, variational sensitivi-
139 ties computed within the same IGA model, and sensitivity-enhanced polynomial chaos regression
140 for geometric UQ remains comparatively unexplored.

141 Accordingly, this paper introduces an IGA-based sensitivity-enhanced polynomial chaos ex-
142 pansion for systems in which geometric uncertainty is represented through a small set of uncertain
143 shape parameters. The proposed approach uses IGA as a unified framework in which geometry,
144 mechanical analysis, and variational sensitivity evaluation are consistently defined. The resulting
145 sensitivities are incorporated into the KKT-based regression problem as derivative information
146 evaluated at selected sensitivity points. This augments response data with mechanically con-
147 sistent derivative information and aims to improve surrogate accuracy and gradient fidelity in
148 data-scarce regimes. The experimental design (ED) is generated by Latin Hypercube Sampling
149 (LHS) [38]. The framework is assessed through four benchmark problems spanning two- and
150 three-dimensional linear elasticity models, nonlinear Neo-Hookean mechanics, and a nonlinear ex-

151 tension with combined geometric and material uncertainty. In the latter case, Poisson’s ratio is
 152 treated as an additional uncertain parameter, while derivative constraints remain restricted to the
 153 geometric variables. The numerical assessment considers response accuracy, gradient accuracy,
 154 and equivalent high-fidelity computational cost. To further evaluate the proposed methodology, a
 155 cost-aware comparison with gradient-enhanced Kriging using central finite-difference gradients is
 156 included as an external derivative-informed benchmark. The main contributions of this study are
 157 summarized as follows:

- 158 • **An isogeometric sensitivity-enhanced polynomial chaos formulation** in which vari-
 159 ational sensitivities computed within the same NURBS-based representation used for ge-
 160 ometry and mechanical analysis are incorporated as derivative information into the PCE
 161 construction.
- 162 • **An application to nonlinear Neo-Hookean mechanics**, including the corresponding
 163 variational sensitivity formulation.
- 164 • **A numerical assessment of response accuracy and gradient fidelity** across four
 165 linear and nonlinear benchmarks, including combined geometric and material uncertainty.
- 166 • **A cost-aware comparison with gradient-enhanced Kriging using central finite-**
 167 **difference gradients**, based on equivalent high-fidelity model evaluations and prescribed
 168 error thresholds.

169 The remainder of this paper is organized as follows. Section 2 reviews the construction of poly-
 170 nomial chaos expansions. Section 3 summarizes constrained PCE formulations used as method-
 171 ological background. Section 4 describes the representation of low-dimensional parametric geo-
 172 metric uncertainty within the IGA framework and the computation of variational sensitivities.
 173 Section 5 presents the proposed IGA-based sensitivity-enhanced PCE formulation. Section 6
 174 presents the numerical examples, including implementation details, reproducibility information,
 175 computational-cost considerations, and performance assessment. Conclusions are drawn in Sec-
 176 tion 7.

2. Polynomial Chaos Expansion

2.1. Formulation of the problem

Consider a mechanical system subjected to static loads, whose spatial domain is defined by geometric parameters (such as lengths, thicknesses, and curvatures) that are uncertain. These uncertainties may arise from the variability in manufacturing processes, load-induced changes, fluctuations in environmental conditions, or long-term service effects. Therefore, in this work, the uncertainty affecting the system is modeled as aleatory, reflecting inherent variability. The uncertain geometric parameters are modeled by a set of independent random variables $\boldsymbol{\mathcal{X}} = (\mathcal{X}_1, \mathcal{X}_2, \dots, \mathcal{X}_M)$, where M denotes the number of uncertain parameters, each characterized by a known probability density function (PDF) $f_{\mathcal{X}_i}(x_i)$, $i = 1, \dots, M$. If dependent geometric parameters are present, they can be mapped to an equivalent set of independent random variables through a suitable iso-probabilistic transformation. A realization of $\boldsymbol{\mathcal{X}}$ is denoted by $\boldsymbol{x} = (x_1, x_2, \dots, x_M)$. Hereafter, subscripts refer to components of the random vector, whereas superscripts in parentheses denote realizations. To evaluate the structural behavior of this system, a set of partial differential equations (PDEs) governing the physics must be solved. To obtain an approximate solution to these PDEs through a numerical model $\mathcal{M}(\boldsymbol{x})$, the Finite Element Method (FEM) [39], Boundary Element Method (BEM) [40], Isogeometric Analysis (IGA) [10], or any of their variations can be applied. Note that the model $\mathcal{M}(\boldsymbol{x})$ depends explicitly on the realizations of the uncertain geometric parameters $\boldsymbol{x}$.

The output of the model, denoted by $\boldsymbol{y}$, represents the system response (such as displacements, stresses, or strains) and is defined as the mapping

$$\mathcal{M}(\boldsymbol{x}) : \boldsymbol{y} = m(\boldsymbol{x}), \quad (1)$$

where m denotes the response operator that maps realizations of the uncertain geometric parameters $\boldsymbol{x}$ to the system response $\boldsymbol{y}$. Moreover, it is important to note that the behavior of the system is influenced by the randomness of the input vector $\boldsymbol{\mathcal{X}}$ during the mapping with m . Consequently, the response of the system is also subject to uncertainty. For the case of scalar outputs, the system response uncertainty is represented by a random variable $\mathcal{Y}$.

Solving the numerical model $\mathcal{M}(\boldsymbol{x})$ of Eq. (1) for multiple realizations of the uncertain geometric parameters can be computationally prohibitive, particularly when high-fidelity discretizations

such as FEM or IGA are employed. Surrogate modeling techniques such as Polynomial Chaos Expansion (PCE) [18] therefore provide an effective alternative for uncertainty quantification.

In the next subsection, the approximate representation of the model response $\mathcal{M}(\mathbf{x})$ is introduced using Polynomial Chaos Expansion.

2.2. Polynomial Chaos Expansion

Polynomial Chaos Expansion (PCE) [18] provides a well-established framework for approximating the response of complex systems by representing the output as a series of orthogonal polynomial basis functions defined in a probabilistic space. This technique is particularly advantageous when the use of Monte Carlo simulation is prohibitively expensive. To construct the polynomial chaos expansion, the physical random variables $\mathcal{X}$ are mapped to a set of independent canonical random variables, hereafter referred to as stochastic germs, $\Theta = (\Theta_1, \dots, \Theta_M)$, through an isoprobabilistic transformation. The PCE is then formulated in terms of these stochastic germs, ensuring that the polynomial basis functions are orthonormal with respect to known reference probability measures.

For a scalar stochastic response $\mathcal{Y}$ with finite variance, and assuming measurability with respect to Θ (as ensured by the Doob–Dynkin lemma),

$$\mathcal{Y}(\Theta) = \sum_{\alpha \in \mathbb{N}^M} y_{\alpha} \Psi_{\alpha}(\Theta), \quad (2)$$

where α is a multi-index that defines the polynomial degree in each variable, $y_{\alpha} \in \mathbb{R}$ represents the expansion coefficient associated with the multi-index α , and $\Psi_{\alpha}(\Theta)$ are multivariate orthogonal polynomials.

Since the stochastic germs Θ are assumed to be independent, the multivariate polynomial basis functions are constructed as tensor products of univariate polynomials orthonormal with respect to the probability measure of each Θ_i . In mathematical terms, the multivariate basis functions are defined as

$$\Psi_{\alpha}(\Theta) = \prod_{i=1}^M \phi_{\alpha_i}^{(i)}(\Theta_i), \quad (3)$$

where $\phi_{\alpha_i}^{(i)}(\Theta_i)$ are orthonormal polynomials in the i -th stochastic germ of degree α_i satisfying

$$\int_{\mathcal{D}_{\Theta_i}} \phi_{\alpha_i}^{(i)}(\theta_i) \phi_{\beta_i}^{(i)}(\theta_i) f_{\Theta_i}(\theta_i) d\theta_i = \delta_{\alpha_i \beta_i}. \quad (4)$$

Here, $\mathcal{D}_{\Theta_i}$ is the domain of the stochastic germ Θ_i , $f_{\Theta_i}(\theta_i)$ is its probability density function, and

229 θ_i denotes a realization of Θ_i . Moreover, $\delta_{\alpha_i\beta_i}$ is the Kronecker delta, which equals one if $\alpha_i = \beta_i$
 230 and zero otherwise.

231 To make the expansion computationally feasible, it is truncated to a finite number of terms P
 232 as

$$\mathcal{Y}^{\text{PCE}}(\boldsymbol{\Theta}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} y_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\Theta}), \quad (5)$$

233 where the truncation set $\mathcal{A}$ follows

$$\mathcal{A}_{M,p_p} = \{\boldsymbol{\alpha} \in \mathbb{N}^M : \|\boldsymbol{\alpha}\|_1 \leq p_p\}. \quad (6)$$

234 Here, $\mathcal{Y}^{\text{PCE}}(\boldsymbol{\Theta})$ is the truncated PCE approximation of the system response, $\mathcal{A}_{M,p_p}$ defines the
 235 retained polynomial terms, p_p is the maximum polynomial degree, and $\|\cdot\|_1$ denotes the L^1 norm.
 236 Only terms whose total degree $\|\boldsymbol{\alpha}\|_1$ is less than or equal to p_p are retained, although other
 237 truncation rules may also be used.

238 The number of terms in the truncated expansion P is given by

$$P = \frac{(M + p_p)!}{M!p_p!}. \quad (7)$$

239 Notably, the truncated expansion introduces an error ϵ , that is

$$\mathcal{Y} = \mathcal{Y}^{\text{PCE}} + \epsilon = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} y_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\Theta}) + \epsilon. \quad (8)$$

240 In practice, the experimental design is generated in the physical space $\boldsymbol{x}^{(i)}$, and the corre-
 241 sponding stochastic germ realizations $\boldsymbol{\Theta}^{(i)}$ are obtained through the isoprobabilistic transforma-
 242 tion. From Eq. (8), the coefficients $\boldsymbol{y}_{\boldsymbol{\alpha}}$ are determined by minimizing the discrepancy between
 243 the PCE surrogate and model evaluations from an experimental design (ED) $\{\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)}\}_{i=1}^{n_{\text{sim}}}$, where
 244 $\boldsymbol{y}^{(i)} = \mathcal{M}(\boldsymbol{x}^{(i)})$ are realizations of $\mathcal{Y}$. This is because, from a statistical perspective, the truncated
 245 PCE in Eq. (5) can be interpreted as a linear regression model with an intercept. Then, the
 246 coefficients $\boldsymbol{y}_{\boldsymbol{\alpha}}$ can be determined using ordinary least squares (OLS), that is

$$\boldsymbol{y}_{\boldsymbol{\alpha}} = (\boldsymbol{\Psi}^T \boldsymbol{\Psi})^{-1} \boldsymbol{\Psi}^T \boldsymbol{y}^D, \quad (9)$$

247 where $\boldsymbol{\Psi}$ is the regression matrix containing evaluations of the polynomial basis functions at the

248 stochastic germ realizations $\Theta^{(i)}$, and $\mathbf{y}^D = [y^{(1)}, \dots, y^{(n_{\text{sim}})}]^T$ is the vector of model responses.
 249 Once the coefficients $\mathbf{y}_\alpha$ are found, statistical moments of the output can be estimated directly
 250 from the expansion, which makes UQ tasks straightforward [22].

251 In this work, uniformly distributed geometric parameters lead to the use of Legendre polyno-
 252 mial basis functions, although the formulation remains general with respect to the choice of input
 253 distributions. As indicated by Eq. (7), the number of PCE terms P increases rapidly with the in-
 254 put dimension M and maximum polynomial degree p_p , increasing the number of model evaluations
 255 required for a stable regression problem. Sparse regression methods such as Least Angle Regres-
 256 sion (LAR) [21] can alleviate this requirement by identifying a reduced active polynomial basis.
 257 Nevertheless, response-only sparse PCE may remain sample-demanding for geometry-dependent
 258 responses, motivating the incorporation of derivative information into the surrogate construction.

259 3. Constrained Polynomial Chaos Regression

260 One way to enrich PCE is to impose additional information through constrained regression.
 261 Building on the PCE framework from Section 2.2, Physics-Informed Polynomial Chaos Expansion
 262 (PC²) (also referred to as constrained PCE) [27] incorporates operator-based constraints derived
 263 from governing equations and boundary conditions into the coefficient estimation. This section
 264 summarizes the original operator-based PC² formulation as methodological background for the
 265 sensitivity-enhanced formulation introduced later.

266 Consider that, for a given realization of the input parameters, the system response $\mathbf{y}(\mathbf{x})$ satisfies
 267 a PDE of the form

$$\mathcal{L}(\mathbf{x}, \mathbf{y}(\mathbf{x})) = f(\mathbf{x}), \quad \mathbf{x} \in \mathcal{D}, \quad (10)$$

268 with boundary conditions $\mathcal{B}(\mathbf{x}, \mathbf{y}(\mathbf{x})) = g(\mathbf{x})$ for $\mathbf{x} \in \partial\mathcal{D}$, where $\mathcal{L}$ and $\mathcal{B}$ are differential operators,
 269 and f and g are prescribed forcing terms.

270 The PC² coefficients $\mathbf{y}_\alpha$ are found by solving a constrained extension of the OLS problem in
 271 Eq. (9), that is,

$$\min_{\mathbf{y}_\alpha} \|\mathbf{y}^D - \Psi \mathbf{y}_\alpha\|^2 \quad \text{subject to} \quad \mathbf{A} \mathbf{y}_\alpha = \mathbf{c}, \quad (11)$$

272 where $\mathbf{A}$ encompasses the PDE and boundary condition constraints, and $\mathbf{c}$ contains the corre-
 273 sponding prescribed values.

274 Note that constructing the $\mathbf{A}$ matrix requires derivatives of the PCE model. In the original

PC² formulation [27], these derivatives are evaluated analytically by differentiating the polynomial chaos basis functions. For example, when first-order derivative information is required, the gradient of the PCE surrogate with respect to the j -th stochastic input is expressed as a linear combination of the derivatives of the polynomial basis, that is,

$$\frac{\partial \mathcal{Y}^{\text{PCE}}(\boldsymbol{\Theta})}{\partial \Theta_j} = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \frac{\partial \Psi_{\alpha}(\boldsymbol{\Theta})}{\partial \Theta_j}. \quad (12)$$

More generally, when derivatives are expressed with respect to physical input variables rather than standardized stochastic germs, the corresponding scaling must be included. For the uniformly distributed input variables considered in this work, the transformation from x_j to Θ_j is affine. Consequently, the chain rule reduces to a constant scaling factor. Therefore, the n -th order derivative of a PCE model with respect to a physical variable x_j satisfies [27]

$$\frac{\partial^n \mathcal{Y}^{\text{PCE}}}{\partial x_j^n} = \frac{\partial^n}{\partial \Theta_j^n} \left[\sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\boldsymbol{\Theta}) \right] \Delta_{\Gamma,j}^n = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \frac{\partial^n \Psi_{\alpha}(\boldsymbol{\Theta})}{\partial \Theta_j^n} \Delta_{\Gamma,j}^n. \quad (13)$$

Here, $\Delta_{\Gamma,j}$ accounts for the scaling between the physical variable x_j and the standardized germ Θ_j . For Legendre polynomials defined on $\Theta_j \in [-1, 1]$ and a uniformly distributed input $x_j \sim \mathcal{U}(\underline{x}_j, \bar{x}_j)$, this factor is given by

$$\Delta_{\Gamma,j} = \frac{2}{\bar{x}_j - \underline{x}_j}. \quad (14)$$

This analytical structure enables differential constraints to be incorporated directly within the PC² framework. Accordingly, the matrix $\mathbf{A}$ represents operator-based constraints obtained by evaluating the boundary operator $\mathcal{B}$ and the PDE operator $\mathcal{L}$ directly on the PCE basis functions $\boldsymbol{\Psi}$. For details, the reader is referred to [27]. The proposed formulation introduced in Section 5 retains the underlying KKT-based regression structure, but uses IGA-derived variational sensitivities as derivative information instead of operator-based PDE and boundary-condition information.

The solution of Eq. (11) is obtained via the Karush–Kuhn–Tucker (KKT) conditions,

$$\begin{bmatrix} \boldsymbol{\Psi}^{\top} \boldsymbol{\Psi} & \mathbf{A}^{\top} \\ \mathbf{A} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{y}_{\alpha} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\Psi}^{\top} \mathbf{y}^D \\ \mathbf{c} \end{bmatrix}, \quad (15)$$

where $\boldsymbol{\lambda}$ are Lagrange multipliers. This formulation minimizes the squared discrepancy with the experimental data while incorporating the operator-based constraints through the KKT system.

To solve Eq. (15), the original PC² framework employs three discrete sets of samples, namely the experimental design, boundary points, and virtual points. The experimental design (ED) $\{\boldsymbol{x}^{(i)}, y^{(i)}\}_{i=1}^{n_{\text{sim}}}$ is obtained from direct model evaluations of Eq. (1). These evaluations populate the regression matrix $\boldsymbol{\Psi}$ of Eq. (9) and link the surrogate to the responses of the underlying model. Boundary points $\{\boldsymbol{x}^{(b)}\}_{b=1}^{n_{\text{BC}}}$ are prescribed locations on $\partial\mathcal{D}$ where Dirichlet/Neumann boundary conditions are enforced. Virtual points $\{\boldsymbol{x}^{(v)}\}_{v=1}^{n_{\text{V}}}$ correspond to artificial collocation points in $\mathcal{D}$ where the PDE residual is enforced without requiring additional model evaluations. The last two groups of points, n_{BC} and n_{V} , populate the constraint matrix $\boldsymbol{A}$ in the KKT system of Eq. (15).

The sizes of these three sets ($n_{\text{sim}}, n_{\text{BC}}, n_{\text{V}}$) can be selected independently, subject to the necessary counting condition

$$P \leq n_{\text{sim}} + n_{\text{BC}} + n_{\text{V}}, \quad (16)$$

where P is the number of PCE terms from Eq. (7). This counting condition alone does not guarantee full rank of the resulting algebraic system.

The constrained regression and sparse PCE components used in this work were implemented using UQPy [41]. The following section introduces the IGA formulation used to compute geometry-consistent variational sensitivities, which are subsequently incorporated as derivative information into the proposed sensitivity-enhanced PCE formulation.

4. Isogeometric analysis

The previous section introduced the operator-based PC² formulation as the constrained-regression background for the proposed methodology. In the present work, the additional derivative information used to enrich the PCE surrogate is instead provided by geometry-consistent variational sensitivities computed within an isogeometric analysis framework. For the low-dimensional parametric geometric uncertainty considered here, IGA provides a unified NURBS-based setting for geometry parameterization, mechanical analysis, and sensitivity evaluation. Accordingly, Section 4.1 introduces the geometric representation, Section 4.2 presents the corresponding linear and nonlinear mechanical formulations, and Section 4.3 derives the geometry-dependent variational sensitivities subsequently incorporated into the sensitivity-enhanced PCE formulation.

323 4.1. NURBS basis functions

324 Isogeometric Analysis (IGA) generalizes the finite element method (FEM) by employing Computer-
 325 Aided Design (CAD) basis functions for both geometric representation and field approxima-
 326 tion [10, 11]. By using Non-Uniform Rational B-Spline (NURBS) basis functions, IGA preserves
 327 exact CAD geometry while providing smooth solution spaces, in contrast to standard finite element
 328 analysis (FEA), where the geometry is typically approximated by polynomial shape functions [42].
 329 This unification of geometry and analysis improves geometric fidelity and can increase accuracy
 330 for a given number of degrees-of-freedom [43]. Although NURBS are most commonly used, alter-
 331 native spline technologies such as T-splines [44], S-splines [45], and LR-splines [46] have also been
 332 developed within the IGA framework. These spline-based geometric descriptions are defined in
 333 the parametric space $\tilde{\Omega}$ through control points and knot vectors Ξ , given by

$$\Xi = \{\xi_1, \xi_2, \dots, \xi_{n+p+1}\}, \quad (17)$$

334 where ξ_i define the knots, p is the polynomial degree, n denotes the number of basis functions,
 335 and repeated knots reduce the inter-element continuity to C^{p-k} , where k is the knot multiplicity.
 336 Note that the knot vector contains $n + p + 1$ non-decreasing entries.

337 B-Spline basis functions are recursively calculated from knot vectors depending on their poly-
 338 nomial degree. For $p = 0$, the expression for the one-dimensional B-Spline functions reads

$$N_{i,0}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1}, \\ 0 & \text{otherwise.} \end{cases} \quad (18)$$

339 For all higher degrees, the basis functions are constructed recursively following the Cox-de
 340 Boor formulas [42, 47]

$$N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi), \quad (19)$$

341 where the fractions are set to zero if their denominator is zero.

342 While B-splines can be used as basis functions within a finite element framework, employing
 343 their rational counterpart (which considers the inclusion of weights) offers advantages, including
 344 the exact representation of conic sections (e.g., circles). For one-dimensional descriptions, the

345 NURBS basis functions are defined as

$$R_{i,p}(\xi) = \frac{w_i N_{i,p}(\xi)}{W(\xi)}, \quad 1 \leq i \leq n_{\text{cp}}, \quad \text{with} \quad W(\xi) = \sum_{\hat{i}=1}^{n_{\text{cp}}} w_{\hat{i}} N_{\hat{i},p}(\xi), \quad (20)$$

346 where n_{cp} is the total number of NURBS control points, $w_i > 0$ are weight factors, and $N_{i,p}$ are
 347 B-spline basis functions of degree p (see Eq. (19)). For open knot vectors, NURBS basis functions
 348 are interpolatory only at the ends of the parametric interval and are generally non-interpolatory at
 349 interior knots. These smoothness and continuity properties make NURBS particularly suitable for
 350 Galerkin-based isogeometric discretizations. As a result, NURBS enable the exact representation
 351 of important CAD entities, such as conic sections, and provide a flexible representation for complex
 352 geometries. NURBS curves $\mathbf{C}(\xi, \mathbf{x})$, surfaces $\mathbf{S}(\xi, \eta, \mathbf{x})$ and volumes $\mathbf{V}(\xi, \eta, \zeta, \mathbf{x})$ are respectively
 353 described by

$$\begin{aligned} \mathbf{C}(\xi, \mathbf{x}) &= \sum_{i=1}^n R_{i,p}(\xi) \mathbf{P}_i(\mathbf{x}), \\ \mathbf{S}(\xi, \eta, \mathbf{x}) &= \sum_{i=1}^n \sum_{j=1}^m R_{i,p}(\xi) R_{j,q}(\eta) \mathbf{P}_{i,j}(\mathbf{x}), \\ \mathbf{V}(\xi, \eta, \zeta, \mathbf{x}) &= \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^l R_{i,p}(\xi) R_{j,q}(\eta) R_{k,r}(\zeta) \mathbf{P}_{i,j,k}(\mathbf{x}), \end{aligned} \quad (21)$$

354 where $\mathbf{x}$ represents the uncertain geometric parameters (such as lengths, thicknesses, and radii)
 355 and $\mathbf{P}(\mathbf{x})$ stores the control-point coordinates. Here, n , m , and l denote the number of NURBS
 356 basis functions in the first, second, and third parametric directions, respectively, while p , q , and
 357 r denote the corresponding polynomial orders. The total number of control points is therefore
 358 given by $n_{\text{cp}} = nml$ for a three-dimensional geometry (and analogously $n_{\text{cp}} = nm$ and $n_{\text{cp}} = n$
 359 for surfaces and curves, respectively). Note that η denotes the second parametric coordinate,
 360 associated with the knot vector $\mathbf{H}$, while ζ denotes the third parametric coordinate, associated
 361 with the knot vector $\mathbf{Z}$. The knot vectors $\mathbf{H}$ and $\mathbf{Z}$ are defined analogously to Eq. (17).

362 Geometric uncertainty is therefore introduced directly through the dependence of the control-
 363 point coordinates $\mathbf{P}(\mathbf{x})$ on the uncertain parameters $\mathbf{x}$. This parameterization allows the resulting
 364 geometric variability and structural response to be treated consistently within the same isogeomet-
 365 ric framework. The corresponding structural response can then be evaluated consistently within
 366 the same analysis framework, as detailed in the next section.

367 4.2. Structural response

368 4.2.1. Linear behavior

369 The computational frameworks employed for the IGA and FEA methods are closely related
 370 when applied to linear elasticity problems such as the one examined in this paper. In the context
 371 of isogeometric analysis, the discretization process involves utilizing NURBS basis functions, as
 372 defined in the previous section. Consequently, the starting point for defining the field responses,
 373 analogous to standard FEA formulations, is the Weak Form of Equilibrium

$$R(\mathbf{u}, \mathbf{v}, \mathbf{x}) = \int_{\Omega(\mathbf{x})} \boldsymbol{\varepsilon}(\mathbf{u}, \mathbf{x}) : \mathbb{C} : \boldsymbol{\varepsilon}(\mathbf{v}, \mathbf{x}) dV - \int_{\Omega(\mathbf{x})} \mathbf{b} \cdot \mathbf{v} dV - \int_{\Gamma_t(\mathbf{x})} \mathbf{t} \cdot \mathbf{v} dA = 0, \quad (22)$$

374 where $R(\mathbf{u}, \mathbf{v}, \mathbf{x})$ represents the residual form of the equilibrium equation, $\mathbf{x}$ denotes the uncertain
 375 geometric parameters, $\boldsymbol{\varepsilon}$ is the linear strain tensor, and $\mathbb{C}$ is the fourth-order elasticity tensor. $\mathbf{u}$
 376 and $\mathbf{v}$ denote the displacement and virtual displacement fields, respectively, while $\mathbf{b}$ and $\mathbf{t}$ are
 377 the prescribed body-force and traction vectors. Here, $\Gamma_t(\mathbf{x}) \subset \partial\Omega(\mathbf{x})$ denotes the Neumann
 378 boundary on which tractions are prescribed. The physical space domain $\Omega(\mathbf{x})$ is discretized using
 379 sub-domains called elements or knot-spans Ω_e that are defined in the parametric space $\tilde{\Omega}$ by the
 380 structure of the knot vectors (i.e., Ξ and $\mathbf{H}$ in two-dimensional cases, and Ξ , $\mathbf{H}$ and $\mathbf{Z}$ for three-
 381 dimensional systems). Note that uncertainty in the geometric parameters affects the physical
 382 domain $\Omega(\mathbf{x})$. This dependence implies that geometric uncertainty enters the governing equations
 383 through the spatial domain itself.

384 The discretization of the Weak Form of Eq. (22) is performed utilizing NURBS basis functions
 385 defined in Eq. (20). For the sake of simplicity, derivations for the two-dimensional case are
 386 considered from this point onwards. However, it is important to note that the expressions can be
 387 readily extended to the three-dimensional case. Since the isoparametric concept is applied and
 388 the interpolation scheme is performed in a Galerkin sense, the geometry, displacement field, and
 389 its corresponding test functions, are discretized by the same basis functions, that is

$$\begin{aligned} \mathbf{X}^h(\mathbf{x}) &= \sum_{i=1}^{n_{cp}^e} R_i(\xi, \eta) \mathbf{P}_i(\mathbf{x}) = \mathbf{N} \mathbf{P}_e(\mathbf{x}), & \mathbf{u}^h(\mathbf{x}) &= \sum_{i=1}^{n_{cp}^e} R_i(\xi, \eta) \mathbf{u}_i(\mathbf{x}) = \mathbf{N} \mathbf{u}_e(\mathbf{x}), \\ \mathbf{v}^h &= \sum_{i=1}^{n_{cp}^e} R_i(\xi, \eta) \mathbf{v}_i = \mathbf{N} \mathbf{v}_e, \end{aligned} \quad (23)$$

where $\mathbf{X}^h(\mathbf{x})$, $\mathbf{u}^h(\mathbf{x})$ and $\mathbf{v}^h$ represent approximations of geometry, displacements, and test functions, respectively. $\mathbf{N}$ is the matrix of shape functions, and n_{cp}^e is the number of control points of an element Ω_e . $\mathbf{P}_e(\mathbf{x})$, $\mathbf{u}_e(\mathbf{x})$, and $\mathbf{v}_e$ are the control-point matrix, displacements, and test functions, per element, respectively. Here, uncertainty associated with the geometric parameters $\mathbf{x}$ is propagated to the geometry $\mathbf{X}^h(\mathbf{x})$, and the displacement field $\mathbf{u}^h(\mathbf{x})$.

Using this matrix notation, the symmetric linear strains can be approximated by,

$$\boldsymbol{\varepsilon}(\mathbf{u}^h, \mathbf{x}) = \sum_{i=1}^{n_{cp}^e} \mathbf{B}_i(\mathbf{x}) \mathbf{u}_i(\mathbf{x}) = \mathbf{B}(\mathbf{x}) \mathbf{u}_e(\mathbf{x}) \quad \text{and} \quad \boldsymbol{\varepsilon}(\mathbf{v}^h, \mathbf{x}) = \sum_{i=1}^{n_{cp}^e} \mathbf{B}_i(\mathbf{x}) \mathbf{v}_i = \mathbf{B}(\mathbf{x}) \mathbf{v}_e, \quad (24)$$

with the strain-displacement matrix $\mathbf{B}(\mathbf{x})$ and the matrix of shape functions $\mathbf{N}$ given by

$$\mathbf{B}(\mathbf{x}) = \begin{bmatrix} R_{1,X} & 0 & \dots & R_{n_{cp}^e,X} & 0 \\ 0 & R_{1,Y} & \dots & 0 & R_{n_{cp}^e,Y} \\ R_{1,Y} & R_{1,X} & \dots & R_{n_{cp}^e,Y} & R_{n_{cp}^e,X} \end{bmatrix} \quad \text{and} \quad \mathbf{N} = \begin{bmatrix} R_1 & 0 & \dots & R_{n_{cp}^e} & 0 \\ 0 & R_1 & \dots & 0 & R_{n_{cp}^e} \end{bmatrix}. \quad (25)$$

As observed in Eq. (25), the shape-function matrix $\mathbf{N}$ is composed of the NURBS basis functions defined in Eq. (20). Moreover, observe that $\mathbf{B}(\mathbf{x})$ is obtained from the derivatives of the shape functions with respect to the global spatial coordinates X and Y . As in standard FEM the strain-displacement matrix is also dependent on $\mathbf{x}$.

Therefore, the discretized matrix form of the Weak Equilibrium equation is given by

$$R_e(\mathbf{x}) = \mathbf{v}_e^T \mathbf{R}_e(\mathbf{x}) = \mathbf{v}_e^T \left[\left(\int_{\Omega_e(\mathbf{x})} \mathbf{B}^T(\mathbf{x}) \mathbf{C} \mathbf{B}(\mathbf{x}) dV \right) \mathbf{u}_e(\mathbf{x}) - \int_{\Omega_e(\mathbf{x})} \mathbf{N}^T \mathbf{b} dV - \int_{\Gamma_{t,e}(\mathbf{x})} \mathbf{N}^T \mathbf{t} dA \right], \quad (26)$$

where R_e is the residual of the elemental equilibrium equation, $\mathbf{R}_e$ represents the elemental equilibrium residual vector, and $\mathbf{C}$ is the constitutive matrix, which characterizes the material properties. Here, $\Gamma_{t,e}(\mathbf{x}) = \partial\Omega_e(\mathbf{x}) \cap \Gamma_t(\mathbf{x})$ denotes the portion of the element boundary on which tractions are prescribed.

As in standard finite element analysis, the IGA-discretized weak form, Eq. (26), can also be cast into the standard matrix form as, excluding the trivial solution $\mathbf{v} = \mathbf{0}$,

$$\bigcup_{e=1}^{n_{el}} [\mathbf{K}_e(\mathbf{x}) \mathbf{u}_e(\mathbf{x}) - \mathbf{f}_e] = \mathbf{K}(\mathbf{x}) \mathbf{u}(\mathbf{x}) - \mathbf{F} = \mathbf{0}, \quad (27)$$

where $\mathbf{K}_e(\mathbf{x})$ is the element stiffness matrix, $\mathbf{u}_e(\mathbf{x})$ is the element displacement vector, and $\mathbf{f}_e$ is the element force vector. $\bigcup_{e=1}^{n_{\text{el}}}$ represents a union operation over all n_{el} elements in the discretized domain, $\mathbf{K}(\mathbf{x})$ is the stiffness matrix of the system, $\mathbf{F}$ is the force vector, and $\mathbf{u}(\mathbf{x})$ the displacement. Observe how the uncertainty in the geometry $\mathbf{x}$ is propagated to the displacement vector $\mathbf{u}(\mathbf{x})$ and stiffness matrix $\mathbf{K}(\mathbf{x})$. It is important to note that, although the geometry is subject to uncertainty, the loading is prescribed such that the total applied load $\mathbf{F}$ remains unchanged and is therefore treated as independent of the geometric parameters.

The assembly of element-level quantities into their global counterparts follows the standard finite element procedure, with control-point connectivity replacing the nodal connectivity used in conventional FEA [10, 42]. Accordingly, the displacement vector $\mathbf{u}(\mathbf{x})$ contains degrees of freedom associated with the control points rather than nodal displacements, reflecting the generally non-interpolatory character of the NURBS basis in the interior of the parametric domain.

Figure 1 summarizes the geometric mappings underlying the linear and nonlinear formulations considered in this work. The physical domain $\Omega(\mathbf{x})$ is obtained from the parametric domain $\tilde{\Omega}$ through the NURBS representation, while numerical integration is performed by mapping each parametric element to a parent domain for Gauss quadrature. Because the corresponding geometric Jacobian depends explicitly on the uncertain geometric parameters, geometric variability propagates directly through the numerical integration and the resulting structural response. Further details on the standard IGA mappings and assembly procedure can be found in [10].

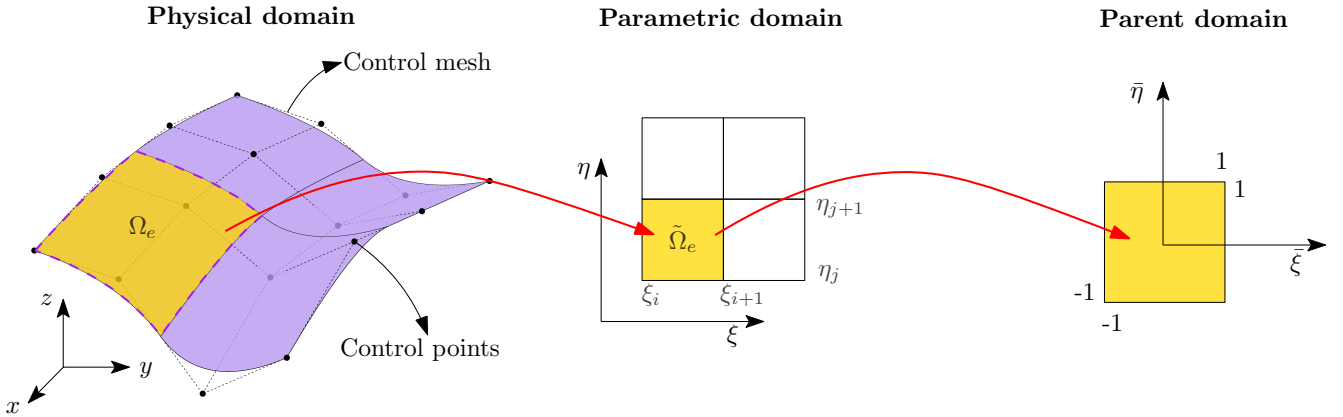


Figure 1: Mappings and integration domains in isogeometric analysis: physical domain Ω (purple), parametric domain $\tilde{\Omega}$, and parent domain used for Gauss quadrature.

4.2.2. Nonlinear behavior

The previous section focused on linear elasticity. The present section extends the formulation to nonlinear material behavior. In this case, the NURBS mapping $\mathbf{X}^h(\mathbf{x})$ (see Eq.(23)) defines the geometry of the reference configuration $\Omega_0(\mathbf{x})$ for each realization of the uncertain geometric parameters $\mathbf{x}$. For a fixed realization $\mathbf{x}$, let $\mathbf{X} \in \Omega_0(\mathbf{x})$ denote the position of a material point in the reference configuration. Note that, throughout this section, the dependence on $\mathbf{x}$ is kept implicit whenever it does not lead to ambiguity. The current position is described by the deformation map $\boldsymbol{\varphi}(\mathbf{X}) = \mathbf{X} + \mathbf{u}(\mathbf{X})$, where $\mathbf{u}$ is the displacement field. The finite-strain kinematic quantities are

$$\begin{aligned} \mathbf{F} &= \frac{\partial \boldsymbol{\varphi}}{\partial \mathbf{X}} = \mathbf{I} + \nabla_{\mathbf{X}} \mathbf{u}, \quad J = \det \mathbf{F} > 0, \\ \mathbf{C} &= \mathbf{F}^\top \mathbf{F}, \quad \mathbf{E} = \frac{1}{2} (\mathbf{C} - \mathbf{I}), \quad I_1 = \text{tr}(\mathbf{C}), \end{aligned} \quad (28)$$

where $\mathbf{F}$ is the deformation gradient, J is its determinant, $\mathbf{C}$ is the right Cauchy–Green tensor, $\mathbf{E}$ is the Green–Lagrange strain tensor, I_1 is the first invariant of $\mathbf{C}$, and $\mathbf{I}$ is the second-order identity tensor.

Different constitutive models may be adopted to characterize the nonlinear elastic response, depending on the material class and the deformation regime of interest. In the present work, a compressible Neo-Hookean model is employed as a simple isotropic hyperelastic constitutive law. The corresponding strain-energy density is given by

$$\mathcal{W}_{\text{NH}}(\mathbf{C}, J) = \frac{\mu}{2} (I_1 - d - 2 \ln J) + \frac{\lambda_L}{2} (J - 1)^2, \quad \mu = \frac{E}{2(1 + \nu)}, \quad \lambda_L = \frac{E\nu}{(1 + \nu)(1 - 2\nu)}, \quad (29)$$

where d is the spatial dimension, E is Young’s modulus, ν is Poisson’s ratio, μ is the shear modulus, and λ_L is the first Lamé parameter. The subscript L distinguishes the Lamé parameter λ_L from the Lagrange multipliers introduced in Section 3.

For a hyperelastic material, the stress measures are obtained from the strain-energy density through standard constitutive relations. Accordingly, the second Piola–Kirchhoff stress $\mathbf{S}$ and the Cauchy stress $\boldsymbol{\sigma}$ are given by

$$\mathbf{S} = 2 \frac{\partial \mathcal{W}_{\text{NH}}}{\partial \mathbf{C}}, \quad \boldsymbol{\sigma} = \frac{1}{J} \mathbf{F} \mathbf{S} \mathbf{F}^\top. \quad (30)$$

448 For the strain-energy density adopted here, these relations yield

$$\mathbf{S} = \mu (\mathbf{I} - \mathbf{C}^{-1}) + \lambda_L J(J-1) \mathbf{C}^{-1} \quad \text{and} \quad \boldsymbol{\sigma} = \frac{\mu}{J} (\mathbf{b} - \mathbf{I}) + \lambda_L (J-1) \mathbf{I}, \quad (31)$$

449 where $\mathbf{b} = \mathbf{F}\mathbf{F}^\top$ is the left Cauchy–Green tensor.

450 As in the linear elasticity formulation, the nonlinear governing equations are obtained from
 451 the weak form of equilibrium based on the principle of virtual work. The variational structure
 452 is preserved, while the infinitesimal strain and linear constitutive relation are replaced by the
 453 finite-strain kinematics and hyperelastic response introduced above. For the virtual displacement
 454 field $\mathbf{v}$ introduced previously, the associated variation of the Green–Lagrange strain tensor is

$$\delta \mathbf{E}(\mathbf{u}; \mathbf{v}) = \frac{1}{2} \left[\mathbf{F}^\top \nabla_{\mathbf{x}} \mathbf{v} + (\nabla_{\mathbf{x}} \mathbf{v})^\top \mathbf{F} \right]. \quad (32)$$

455 Substituting this virtual strain measure into the principle of virtual work yields the nonlinear weak
 456 equilibrium equation at a prescribed load factor $\gamma \in [0, 1]$, which must hold for all kinematically
 457 admissible virtual displacement fields,

$$R_{\text{nl}}(\mathbf{u}, \mathbf{v}, \mathbf{x}; \gamma) = \int_{\Omega_0(\mathbf{x})} \mathbf{S} : \delta \mathbf{E}(\mathbf{u}; \mathbf{v}) \, dV_0 - \gamma \left[\int_{\Omega_0(\mathbf{x})} \mathbf{b}_0 \cdot \mathbf{v} \, dV_0 + \int_{\Gamma_{0,t}(\mathbf{x})} \mathbf{t}_0 \cdot \mathbf{v} \, dA_0 \right] = 0, \quad (33)$$

458 where $\mathbf{b}_0$ is the body-force vector per unit reference volume, $\mathbf{t}_0$ is the prescribed traction vector
 459 on the Neumann boundary $\Gamma_{0,t}(\mathbf{x})$, and dV_0 and dA_0 denote the differential volume and boundary
 460 area in the reference configuration, respectively.

461 Applying the same NURBS-based Galerkin discretization introduced for the linear formulation,
 462 Eq. (33) is discretized as

$$\mathbf{R}_{\text{nl}}(\mathbf{u}, \mathbf{x}; \gamma) = \mathbf{R}_{\text{int}}(\mathbf{u}, \mathbf{x}) - \gamma \mathbf{F}_{\text{ext}} = \mathbf{0}, \quad (34)$$

463 where $\mathbf{u}$ is the global vector of displacement degrees-of-freedom, $\mathbf{R}_{\text{int}}$ is the assembled internal-force
 464 vector, $\mathbf{F}_{\text{ext}}$ is the assembled external-force vector, and $\mathbf{0}$ is the zero vector. Consistently with the
 465 linear formulation, the total external load vector $\mathbf{F}_{\text{ext}}$ is treated as independent of the geometric
 466 parameters.

467 At a fixed value of γ , the residual equation is solved using Newton–Raphson iterations. At

iteration k , the consistent tangent stiffness matrix and the displacement update satisfy

$$\begin{aligned}\mathbf{K}_T^{(k)} &= \left. \frac{\partial \mathbf{R}_{nl}}{\partial \mathbf{u}} \right|_{\mathbf{u}=\mathbf{u}^{(k)}} = \mathbf{K}_{mat}^{(k)} + \mathbf{K}_{geo}^{(k)}, \\ \mathbf{K}_T^{(k)} \Delta \mathbf{u}^{(k)} &= -\mathbf{R}_{nl}(\mathbf{u}^{(k)}, \mathbf{x}; \gamma), \quad \mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \Delta \mathbf{u}^{(k)}.\end{aligned}\tag{35}$$

Here, $\mathbf{K}_T^{(k)}$ is the tangent stiffness matrix, $\mathbf{K}_{mat}^{(k)}$ and $\mathbf{K}_{geo}^{(k)}$ are its material and geometric contributions, $\Delta \mathbf{u}^{(k)}$ is the Newton displacement increment, and k is the iteration index. The converged tangent stiffness matrix is subsequently reused in the nonlinear variational sensitivity problem developed in Section 4.3.

Once either the linear equilibrium problem in Eq. (27) or the nonlinear problem in Eq. (34) is solved, response quantities are evaluated through post-processing and retain their dependence on the geometric parameters through the domain mapping, integration measures, basis-function derivatives, and equilibrium solution. The following subsection introduces the corresponding variational sensitivities, first recalling the linear relations and then developing their nonlinear extension.

4.3. Variational sensitivity analysis for geometry

4.3.1. Linear model

The sensitivity-enhanced PCE formulation requires derivatives of the response with respect to the uncertain geometric parameters. In this work, these derivatives are obtained through variational sensitivity analysis within the IGA framework, exploiting the explicit dependence of the NURBS geometry on the underlying parameters. The required sensitivities reuse information from the structural response analysis, avoiding independent finite-difference response evaluations. Their computation requires access to internal IGA quantities and incurs additional computational cost, as discussed in Section 6.5.

Let $f(\mathbf{u}(\mathbf{x}), \mathbf{x})$ denote a response quantity of interest, where $\mathbf{u}(\mathbf{x})$ is the global vector of displacement degrees of freedom obtained from the discretized equilibrium problem. The function $f(\cdot)$ may represent displacements, stresses, strain-based quantities, or other post-processed responses. The following derivation considers mechanical systems with geometry-dependent domains, whose IGA representation is given by Eq. (23). For clarity, the dependence of the physical geometry on $\mathbf{x}$ is kept implicit hereafter, and the simplified notation $\mathbf{X}$ is adopted.

Following standard results from variational sensitivity analysis [14, 15], the total variation of the response function can be decomposed into contributions associated with changes in the

495 displacement field and changes in the geometry. This leads to the expression

$$\delta f = \delta_u f + \delta_X f = \left[\frac{\partial f}{\partial \mathbf{u}(\mathbf{x})} \right] \delta \mathbf{u}(\mathbf{x}) + \left[\frac{\partial f}{\partial \mathbf{X}} \right] \delta \mathbf{X}. \quad (36)$$

496 Here, $\delta_u f$ represents the indirect contribution arising from variations in the displacement field
 497 induced by geometric changes, whereas $\delta_X f$ captures the direct contribution due to perturbations
 498 of the geometry itself. This decomposition forms the foundation of the variational sensitivity
 499 formulation adopted in this work. Moreover, this decomposition makes explicit that geometric
 500 uncertainty affects the response through both indirect kinematic effects, mediated by the displace-
 501 ment field, and direct geometric effects associated with domain perturbations.

502 To relate the response variations in Eq. (36) to the governing equations, the equilibrium condi-
 503 tion must be enforced for all admissible geometric perturbations. Within the direct differentiation
 504 method (DDM), this is achieved by requiring that the total variation of the Weak Equilibrium
 505 residual vanishes, i.e.,

$$\delta R(\mathbf{u}, \mathbf{v}, \delta \mathbf{u}, \delta \mathbf{X}, \mathbf{x}) = \delta_u R(\mathbf{u}, \mathbf{v}, \delta \mathbf{u}, \mathbf{x}) + \delta_X R(\mathbf{u}, \mathbf{v}, \delta \mathbf{X}, \mathbf{x}) = 0. \quad (37)$$

506 This condition ensures that the equilibrium state is preserved under infinitesimal variations of
 507 the geometry and the associated displacement field. As a result, the response sensitivity can be
 508 derived consistently through direct differentiation, without requiring an adjoint formulation.

509 Using standard Galerkin discretization concepts, the variations in Eq. (37) can be expressed
 510 in discrete form. The variation with respect to the displacement field is approximated as

$$\delta_u R(\mathbf{u}, \mathbf{v}, \delta \mathbf{u}, \mathbf{x}) \approx \delta_u R(\mathbf{u}^h, \mathbf{v}^h, \delta \mathbf{u}^h, \mathbf{x}) = \mathbf{v}^\top \mathbf{K}(\mathbf{x}) \delta \mathbf{u}(\mathbf{x}), \quad (38)$$

511 where $\mathbf{K}(\mathbf{x})$ denotes the global stiffness matrix, which inherits its dependence on the uncertain
 512 geometry through the isogeometric discretization.

513 Similarly, the variation of the Weak Equilibrium residual with respect to geometric changes
 514 gives rise to an additional contribution. This term captures the effect of perturbations in the spatial
 515 domain induced by variations of the control-point coordinates. In discrete form, the geometric
 516 variation is approximated as

$$\delta_X R(\mathbf{u}, \mathbf{v}, \delta \mathbf{X}, \mathbf{x}) \approx \delta_X R(\mathbf{u}^h, \mathbf{v}^h, \delta \mathbf{X}^h, \mathbf{x}) = \mathbf{v}^\top \mathbf{Q}(\mathbf{x}) \delta \mathbf{P}(\mathbf{x}), \quad (39)$$

517 where $\mathbf{Q}(\mathbf{x})$ denotes a geometry-induced pseudo-load matrix, and $\delta\mathbf{P}(\mathbf{x})$ represents variations of
 518 the NURBS control-point coordinates. The matrix $\mathbf{Q}(\mathbf{x})$ represents the contribution of geomet-
 519 ric perturbations to the equilibrium equations through changes in the internal virtual work. For
 520 the loading conditions considered here, the prescribed external load is independent of the uncer-
 521 tain geometry, such that its derivative vanishes and $\mathbf{Q}(\mathbf{x})$ acts as an equivalent geometry-induced
 522 pseudo-load. In the isogeometric setting, this contribution arises from changes in the parametric-
 523 to-physical mapping and involves derivatives of the NURBS basis functions and the stress field.
 524 Such a pseudo-load is specific to geometric uncertainty and does not arise for non-geometric un-
 525 certain parameters, such as material properties or external loads, when the domain remains fixed.
 526 The pseudo-load matrix $\mathbf{Q}(\mathbf{x})$ is obtained through element-wise differentiation of the weak form
 527 with respect to geometric variations, involving the strain–displacement relations, stress measures,
 528 and derivatives of the NURBS basis functions. Since these expressions follow established varia-
 529 tional sensitivity formulations and do not alter the conceptual development, the full derivation
 530 and explicit elemental expressions of $\mathbf{Q}(\mathbf{x})$ are provided in Appendix A.

531 Since the discrete variational equation must hold for all admissible test vectors $\mathbf{v}$, the response
 532 sensitivity with respect to control-point perturbations is obtained as

$$\mathbf{K}(\mathbf{x}) \delta\mathbf{u}(\mathbf{x}) = -\mathbf{Q}(\mathbf{x}) \delta\mathbf{P}(\mathbf{x}) \quad \Rightarrow \quad \delta\mathbf{u}(\mathbf{x}) = -\mathbf{K}^{-1}(\mathbf{x}) \mathbf{Q}(\mathbf{x}) \delta\mathbf{P}(\mathbf{x}) = \mathbf{S}(\mathbf{x}) \delta\mathbf{P}(\mathbf{x}), \quad (40)$$

533 where $\mathbf{S}(\mathbf{x})$ denotes the displacement sensitivity matrix with respect to the control-point coordi-
 534 nates.

535 To relate the control-point variations to the underlying uncertain geometric parameters, the
 536 perturbation of the NURBS control points is expressed through a design-velocity mapping,

$$\delta\mathbf{P}(\mathbf{x}) = \mathbf{D}(\mathbf{x}) \delta\mathbf{x}, \quad (41)$$

537 where $\mathbf{D}(\mathbf{x})$ is the design-velocity matrix that describes how each geometric parameter perturbs
 538 the control-point coordinates.

539 Combining Eqs. (40) and (41), the sensitivity of the displacement field with respect to the
 540 uncertain geometric parameters is obtained as

$$\delta\mathbf{u}(\mathbf{x}) = \mathbf{S}(\mathbf{x}) \mathbf{D}(\mathbf{x}) \delta\mathbf{x}, \quad \Rightarrow \quad \frac{d\mathbf{u}}{d\mathbf{x}} = \mathbf{S}(\mathbf{x}) \mathbf{D}(\mathbf{x}). \quad (42)$$

Here, the total derivative accounts for the implicit dependence of the displacement field on the geometric parameters through the variational problem.

4.3.2. Nonlinear model

The sensitivity equations presented above correspond to the linear equilibrium problem. For nonlinear systems, the same variational framework is applied to the converged equilibrium state obtained after the final load step ($\gamma = 1$). The nonlinear equilibrium formulation introduced in Eq. (34) depends on the uncertain geometric parameters through the geometry. Within the IGA framework, this dependence is represented explicitly by the NURBS control-point coordinates $\mathbf{P} = \mathbf{P}(\mathbf{x})$. Accordingly, at convergence the discrete nonlinear equilibrium equation may be written as

$$\mathbf{R}_{\text{nl}}(\mathbf{u}(\mathbf{x}), \mathbf{P}(\mathbf{x}); \gamma) = \mathbf{0}, \quad (43)$$

where the dependence on the uncertain geometric parameters is introduced through both the converged displacement vector $\mathbf{u}(\mathbf{x})$ and the control-point coordinates $\mathbf{P}(\mathbf{x})$ defining the geometry. Taking the total derivative of Eq. (34) with respect to the uncertain geometric parameters therefore gives

$$\frac{d}{d\mathbf{x}} [\mathbf{R}_{\text{nl}}(\mathbf{u}(\mathbf{x}), \mathbf{P}(\mathbf{x}); \gamma)] = \underbrace{\frac{\partial \mathbf{R}_{\text{nl}}}{\partial \mathbf{u}}}_{\mathbf{K}_T} \frac{d\mathbf{u}(\mathbf{x})}{d\mathbf{x}} + \frac{\partial \mathbf{R}_{\text{nl}}}{\partial \mathbf{P}} \bigg|_{\mathbf{u}} \frac{d\mathbf{P}(\mathbf{x})}{d\mathbf{x}} = \mathbf{0}. \quad (44)$$

Here, $\mathbf{K}_T(\mathbf{x})$ is the consistent tangent stiffness matrix evaluated at the converged equilibrium state. The first term accounts for the implicit dependence of the residual on the geometric parameters through the equilibrium solution, whereas the second term represents the explicit dependence introduced by the geometry through the control-point parameterization. The partial derivative with respect to $\mathbf{P}$ is evaluated while holding the discrete displacement vector $\mathbf{u}$ fixed.

At the converged configuration, this geometric derivative defines the nonlinear geometry-induced pseudo-load matrix as

$$\mathbf{Q}_{\text{nl}}(\mathbf{x}) = \frac{\partial \mathbf{R}_{\text{nl}}}{\partial \mathbf{P}} \bigg|_{\mathbf{u}} = \mathbf{Q}_{\text{int,nl}}(\mathbf{x}) - \mathbf{Q}_{\text{ext,nl}}(\mathbf{x}), \quad (45)$$

where $\mathbf{Q}_{\text{int,nl}}$ and $\mathbf{Q}_{\text{ext,nl}}$ are the geometric derivatives of the assembled internal- and external-force vectors, respectively. The internal contribution accounts for variations of the reference-domain mapping, the integration measure, the nonlinear kinematic operators, and the resulting stress state. The external contribution accounts for any dependence of the assembled external-force vec-

566 tor on the geometry. For the loading conditions considered in this work, the total prescribed load
 567 is independent of the uncertain geometry; consequently, $\mathbf{Q}_{\text{ext, nl}} = \mathbf{0}$. Nevertheless, the external
 568 contribution is retained in Eq. (45) to preserve the generality of the formulation.

569 Using the design-velocity relation from Eq. (41), the nonlinear displacement sensitivity is
 570 obtained from

$$\mathbf{K}_T(\mathbf{x}) \frac{d\mathbf{u}(\mathbf{x})}{d\mathbf{x}} = -\mathbf{Q}_{\text{nl}}(\mathbf{x})\mathbf{D}(\mathbf{x}), \quad \frac{d\mathbf{u}(\mathbf{x})}{d\mathbf{x}} = -\mathbf{K}_T^{-1}(\mathbf{x})\mathbf{Q}_{\text{nl}}(\mathbf{x})\mathbf{D}(\mathbf{x}) = \mathbf{S}_{\text{nl}}(\mathbf{x})\mathbf{D}(\mathbf{x}), \quad (46)$$

571 where

$$\mathbf{S}_{\text{nl}}(\mathbf{x}) = -\mathbf{K}_T^{-1}(\mathbf{x})\mathbf{Q}_{\text{nl}}(\mathbf{x}) \quad (47)$$

572 is the nonlinear displacement sensitivity matrix with respect to the control-point coordinates.
 573 Consequently, the factorized tangent stiffness matrix obtained from the converged equilibrium
 574 problem can be reused to solve the sensitivity equations associated with all geometric parameter
 575 directions. The nonlinear equilibrium analysis is substantially more expensive than in the lin-
 576 ear case, whereas the additional cost associated with the variational sensitivity analysis remains
 577 comparatively modest. The sensitivity of any post-processed response quantity is subsequently
 578 obtained from the general decomposition introduced in Eq. (36). The computational cost asso-
 579 ciated with the variational sensitivity analysis is assessed in Section 6.5. The full derivation and
 580 the explicit elemental expressions of $\mathbf{Q}_{\text{nl}}(\mathbf{x})$ are provided in Appendix A.

581 The variational sensitivity relations derived in this subsection provide the geometry-consistent
 582 derivative information used in the proposed sensitivity-enhanced PCE construction. They quantify
 583 the dependence of the structural response on the uncertain geometric parameters while remaining
 584 tied to the same NURBS parameterization used for the IGA model. In the following section,
 585 these IGA-derived sensitivities are incorporated into the PCE construction, forming the core of
 586 the proposed methodology.

587 5. Proposed strategy

588 5.1. IGA-based sensitivity-enhanced PCE formulation

589 The proposed IGA-based sensitivity-enhanced PCE formulation combines response evaluations
 590 from the experimental design with geometry-consistent sensitivities obtained through variational
 591 sensitivity analysis. The response data define the standard PCE regression residual, while the

IGA-derived sensitivities provide the derivative information used to enhance the polynomial approximation. The same surrogate construction applies whether these quantities are obtained from a linear or nonlinear equilibrium problem.

Let $\{\mathbf{x}^{(s)}\}_{s=1}^{n_s}$ denote the prescribed sensitivity points in the space of uncertain geometric parameters, with the corresponding derivative least-squares problem defined through the matrix $\mathbf{J}$ and vector $\mathbf{s}$. For a selected polynomial chaos space, exact satisfaction of the sensitivity equations, $\mathbf{J}\mathbf{y}_\alpha = \mathbf{s}$, is possible only if $\mathbf{s} \in \text{Range}(\mathbf{J})$. This compatibility condition is not generally guaranteed when sensitivities of a non-polynomial mechanical response are represented within a finite polynomial basis. Accordingly, incompatible sensitivity equations are not imposed as exact equality constraints.

The formulation used in this work is instead defined through the Moore–Penrose solution of the complete KKT system

$$\mathbf{A}_{\text{KKT}} = \begin{bmatrix} \Psi^\top \Psi & \mathbf{J}^\top \\ \mathbf{J} & \mathbf{0} \end{bmatrix}, \quad \mathbf{b}_{\text{KKT}} = \begin{bmatrix} \Psi^\top \mathbf{y}^D \\ \mathbf{s} \end{bmatrix}, \quad (48)$$

with the coefficient and multiplier vectors obtained as

$$\begin{bmatrix} \mathbf{y}_\alpha^* \\ \boldsymbol{\lambda}^* \end{bmatrix} = \mathbf{A}_{\text{KKT}}^+ \mathbf{b}_{\text{KKT}} = \begin{bmatrix} \Psi^\top \Psi & \mathbf{J}^\top \\ \mathbf{J} & \mathbf{0} \end{bmatrix}^+ \begin{bmatrix} \Psi^\top \mathbf{y}^D \\ \mathbf{s} \end{bmatrix}. \quad (49)$$

where $(\cdot)^+$ denotes the Moore–Penrose pseudoinverse. For the Gram-structured KKT system considered here, this solution admits an equivalent hierarchical least-squares interpretation.

Defining the derivative least-squares solution set as

$$\mathcal{C}_s = \arg \min_{\mathbf{c}} \|\mathbf{J}\mathbf{c} - \mathbf{s}\|_2^2, \quad (50)$$

the PCE coefficients satisfy

$$\mathbf{y}_\alpha^* \in \arg \min_{\mathbf{c} \in \mathcal{C}_s} \|\mathbf{y}^D - \Psi\mathbf{c}\|_2^2. \quad (51)$$

Hence, the construction first attains the minimum derivative residual representable within the selected PCE space and subsequently fits the response within the corresponding derivative least-squares solution set, without increasing that minimum derivative residual. The equality-constrained formulation is recovered as the compatible special case $\mathbf{s} \in \text{Range}(\mathbf{J})$, for which the minimum

613 derivative residual is zero.

614 The degree of compatibility between the available sensitivity information and the selected PCE
 615 space is quantified by the relative derivative residual

$$\rho_s = \frac{\|\mathbf{J}\mathbf{y}_\alpha^* - \mathbf{s}\|_2}{\|\mathbf{s}\|_2}. \quad (52)$$

616 For the adopted Moore–Penrose solution, this residual reaches the minimum derivative discrepancy
 617 attainable within the selected polynomial space. A nonzero value of ρ_s therefore indicates finite-
 618 basis incompatibility between the supplied derivative observations and the selected PCE space,
 619 rather than exact interpolation of all supplied sensitivities.

620 The algebraic construction follows the KKT-based formulation introduced for physics-informed
 621 polynomial chaos in Section 3. In the present setting, however, the matrix $\mathbf{J}$ is assembled di-
 622 rectly from derivatives of the polynomial basis rather than from governing equations or boundary-
 623 condition operators. Its rows contain derivatives of the polynomial chaos basis with respect to the
 624 standardized stochastic germs, evaluated at the prescribed sensitivity points, while $\mathbf{s}$ contains the
 625 corresponding IGA-derived sensitivities expressed in the same standardized space.

626 Since the PCE basis is defined in terms of the stochastic germs Θ , the IGA-derived sensitivities
 627 with respect to the physical geometric parameters must be expressed consistently in the same space
 628 before assembling the sensitivity vector $\mathbf{s}$. For the independent uniformly distributed geometric
 629 parameters considered in this work, $x_j \sim \mathcal{U}(\underline{x}_j, \bar{x}_j)$, the affine transformation is

$$x_j = \frac{\bar{x}_j + \underline{x}_j}{2} + \frac{\bar{x}_j - \underline{x}_j}{2}\Theta_j, \quad \Theta_j \in [-1, 1]. \quad (53)$$

630 Therefore, by the chain rule, the physical IGA sensitivity is transformed to the standardized
 631 stochastic space as

$$s_{\Theta_j}^{(s)} = \left. \frac{\partial \mathcal{Y}}{\partial \Theta_j} \right|_{\mathbf{x}=\mathbf{x}^{(s)}} = \left. \frac{\partial \mathcal{Y}}{\partial x_j} \right|_{\mathbf{x}=\mathbf{x}^{(s)}} \frac{\bar{x}_j - \underline{x}_j}{2}. \quad (54)$$

632 Accordingly, the entries of the sensitivity vector are assembled as $s_{(s,j)} = s_{\Theta_j}^{(s)}$, while the corre-
 633 sponding entries of $\mathbf{J}$ are derivatives of the PCE basis with respect to Θ_j . Equivalently, derivatives
 634 with respect to the physical variables may be obtained from derivatives in the standardized space
 635 using the inverse scaling factor $\Delta_{\Gamma,j} = 2/(\bar{x}_j - \underline{x}_j)$, as in the original constrained polynomial chaos
 636 regression formulation [27].

Since each sensitivity point contributes one derivative observation for each uncertain geometric parameter for which variational sensitivity information is available, $\mathbf{s} \in \mathbb{R}^{n_S M}$ and $\mathbf{J} \in \mathbb{R}^{n_S M \times P}$, where M is the number of uncertain geometric parameters and P denotes the number of retained polynomial chaos terms. For the sparse LAR-based variant, P corresponds to the number of active polynomial terms.

The integration of IGA-derived sensitivities into the proposed formulation is illustrated schematically in Figure 2. Starting from a parameterized NURBS-based geometric description, an experimental design (ED) is generated by sampling the uncertain geometric parameter space, e.g. via Latin Hypercube Sampling (LHS), and evaluating the IGA model at n_{sim} realizations. For the same realizations, variational sensitivity analysis reuses information from the IGA solution to compute derivatives of the response with respect to the uncertain geometric parameters. In all numerical examples, the sensitivity points coincide with the experimental-design realizations, so that $n_S = n_{\text{sim}}$. Thus, each model evaluation $\mathbf{x}^{(i)}$ provides both the response value $y^{(i)}$ and the corresponding physical sensitivity vector $\partial \mathcal{Y} / \partial \mathbf{x} \big|_{\mathbf{x}^{(i)}}$. The sensitivity values are transformed according to Eq. (54) before assembling the vector $\mathbf{s}$.

The resulting sensitivity-enhanced PCE surrogate is informed by both response values and local geometry-dependent derivative information. As illustrated in Figure 2, this integrated strategy is intended to improve surrogate accuracy and gradient quality when only a limited number of high-fidelity response evaluations is available. Furthermore, the proposed approach can be combined with sparse regression techniques, such as least-angle regression (LAR).

5.2. Summary of the proposed strategy

Figure 3 summarizes the proposed IGA-based sensitivity-enhanced PCE framework for geometric uncertainty quantification. The individual steps of the methodology are detailed below and follow the structure of the flowchart.

1. Define the isogeometric analysis (IGA) model, including the geometry, parametric space $\tilde{\Omega}$, boundary conditions, material behavior, and the response of interest y .
2. Identify the uncertain geometric parameters and model them as a random vector $\mathbf{x}$ with prescribed probability distributions.
3. Construct the NURBS-based geometry through a parameterized control-point matrix $\mathbf{P}(\mathbf{x})$, providing a consistent NURBS representation of the physical domain for any realization $\mathbf{x}$.

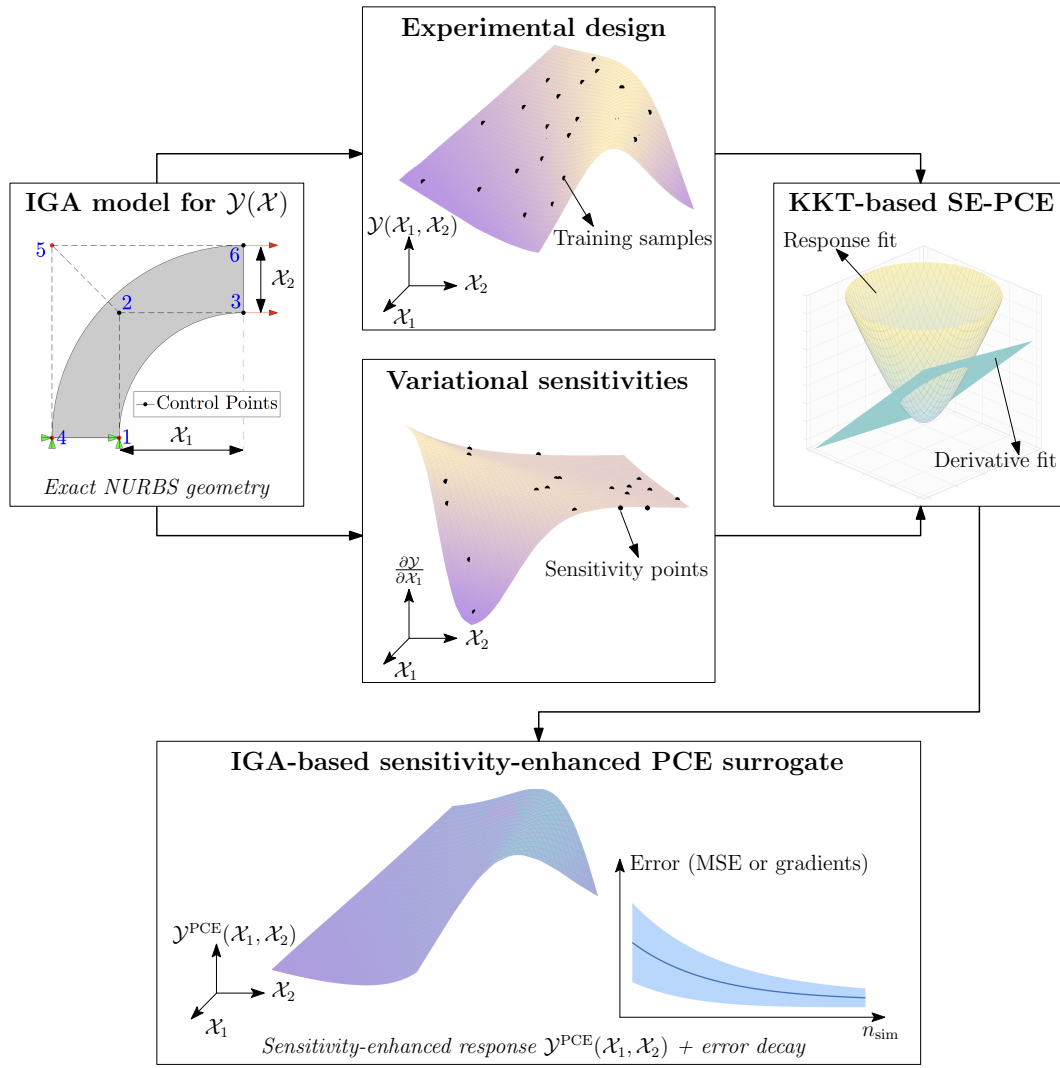


Figure 2: Conceptual scheme of the proposed IGA-based sensitivity-enhanced PCE formulation.

4. Select the polynomial chaos basis, including the polynomial family, maximum order p_p , and multi-index set $\mathcal{A}$. Here, uniform distributions are assumed for the uncertain geometric parameters, leading to Legendre polynomials. A total-order truncation strategy is adopted with candidate maximum polynomial orders between $p_p = 6$ and $p_p = 8$. The choice of this candidate range and the model-selection criterion adopted for each surrogate are detailed in the corresponding numerical examples in Section 6.
5. Generate an experimental design (ED) of size n_{sim} by sampling realizations $\{\mathbf{x}^{(i)}\}_{i=1}^{n_{\text{sim}}}$ from $\mathcal{X}$, for instance using Latin Hypercube Sampling.
 - (a) For each realization $\mathbf{x}^{(i)}$, solve the corresponding linear or nonlinear IGA equilibrium problem to obtain the response $y^{(i)} = \mathcal{M}(\mathbf{x}^{(i)})$ and compute the physical variational sensitivities $\partial \mathcal{Y} / \partial \mathbf{x}$, which are then transformed to the standardized stochastic space

before assembling $\mathbf{s}$.

6. Assemble the response regression matrix Ψ and the derivative matrix $\mathbf{J}$ together with the transformed IGA-derived sensitivity vector $\mathbf{s}$.
7. Construct the IGA-based sensitivity-enhanced PCE surrogate through the Moore–Penrose solution of the complete KKT system in Eq. (49). If the system is ill-conditioned, refine the polynomial basis, enrich the experimental design, or activate sparse regression techniques such as least-angle regression (LAR).
 - (a) Construct the IGA-based sensitivity-enhanced PCE surrogate and evaluate both predictions and gradients.
 - (b) Assess accuracy and sensitivity consistency using verification metrics such as mean squared error, cumulative absolute error, and gradient fidelity.
 - (c) If the prescribed criteria are not satisfied, repeat surrogate construction.

The following section presents numerical results that assess the accuracy and computational behavior of the proposed methodology.

6. Numerical experiments

6.1. Quarter-circular annulus

The first example considers a linear two-dimensional steel quarter-circular annulus. The bottom end of the shape is fixed, and a load of 40 kN is applied at the top end. The material properties are assumed deterministic, with Young’s modulus $E = 2 \times 10^5$ N/mm² and Poisson’s ratio $\nu = 0.3$. Plane stress conditions ($\sigma_{33} = 0$) are assumed. The inner radius r and thickness t are modeled as independent uniform random variables, with $r \sim \mathcal{U}(10, 50)$ mm and $t \sim \mathcal{U}(15, 40)$ mm. The relatively wide parameter ranges are selected to represent pronounced geometric variability and its influence on the stress response. The response of interest is the maximum stress triaxiality σ_{ST} . Stress triaxiality is a physically meaningful indicator of the stress state and plays a central role in the characterization of damage mechanisms and fracture initiation in ductile materials [48, 49, 50].

By definition, the stress triaxiality $\sigma_{\text{ST}}(\mathbf{x})$ is given by the ratio of the hydrostatic stress $\sigma_{\text{M}}(\mathbf{x})$ to the von Mises equivalent stress $\sigma_{\text{V}}(\mathbf{x})$, that is,

$$\sigma_{\text{ST}}(\mathbf{x}) = \frac{\sigma_{\text{M}}(\mathbf{x})}{\sigma_{\text{V}}(\mathbf{x})}, \quad \sigma_{\text{M}}(\mathbf{x}) = \frac{1}{3} \text{tr}(\boldsymbol{\sigma}(\mathbf{x})), \quad \sigma_{\text{V}}(\mathbf{x}) = \sqrt{3J_2(\mathbf{x})}, \quad (55)$$

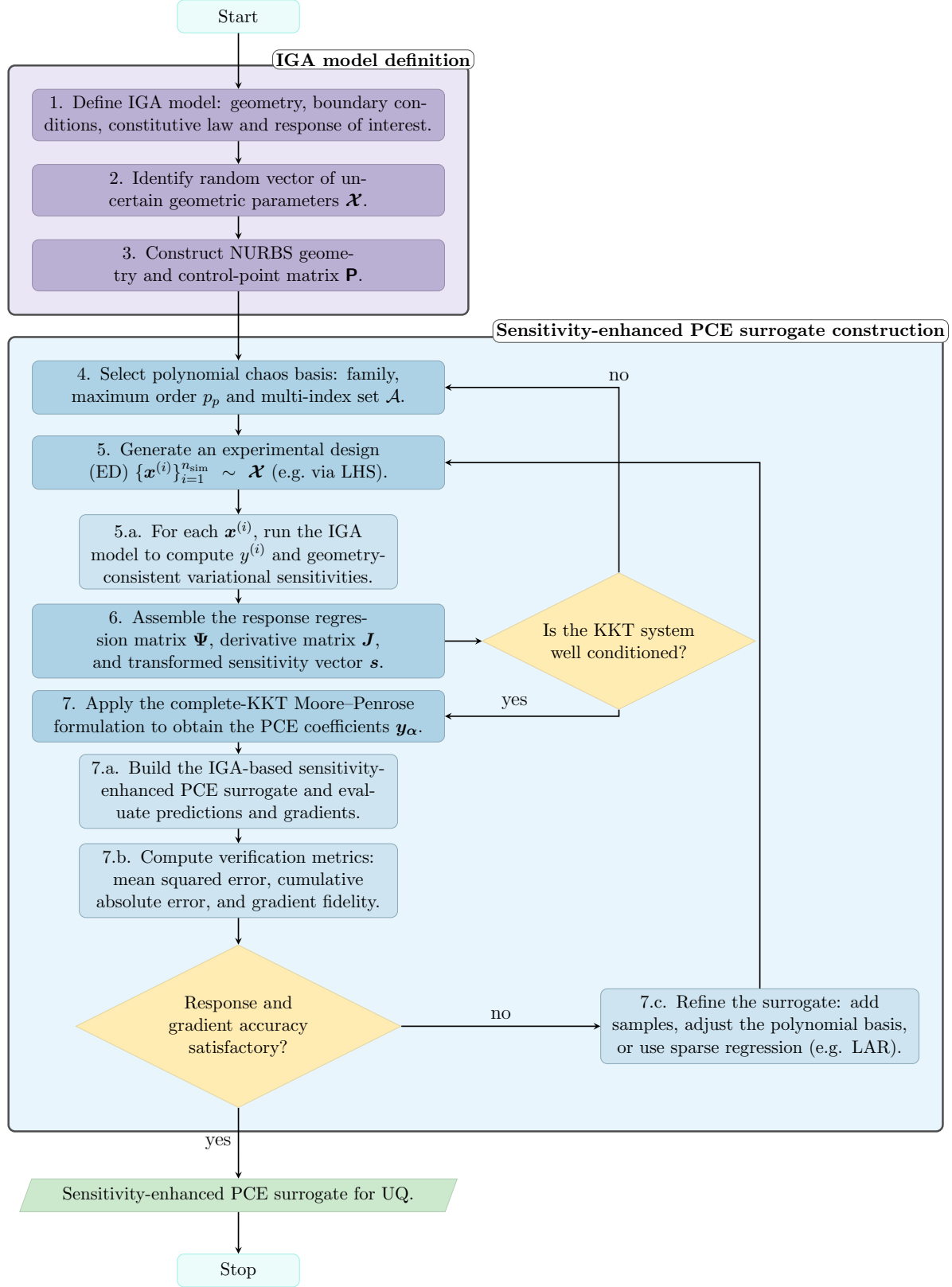


Figure 3: Flowchart of the proposed IGA-based sensitivity-enhanced PCE framework for geometric uncertainty quantification.

705 where $\boldsymbol{\sigma}$ denotes the Cauchy stress tensor and J_2 is the second invariant of the deviatoric stress
 706 tensor.

707 The objective of this example is twofold: (i) to isolate the effect of geometric uncertainty on a
 708 stress-based response quantity, and (ii) to assess the ability of the proposed IGA-based sensitivity-
 709 enhanced PCE formulation to improve response accuracy in a minimal and controlled setting.
 710 Because stress triaxiality depends on the spatial stress distribution, it provides a suitable quantity
 711 of interest for assessing both response and geometry-dependent sensitivity predictions. The spatial
 712 location of the maximum stress triaxiality was monitored across the uncertainty domain, and no
 713 relevant switching of the active maximum was observed. Accordingly, the reported sensitivities
 714 correspond to regions in which the active maximum remains locally unique and varies continuously
 715 with the geometric parameters. A spatial-refinement study was also performed for the quantity
 716 of interest and its geometric sensitivities. The results confirmed that the surrogate comparisons
 717 reported below are not governed by unresolved spatial discretization errors.

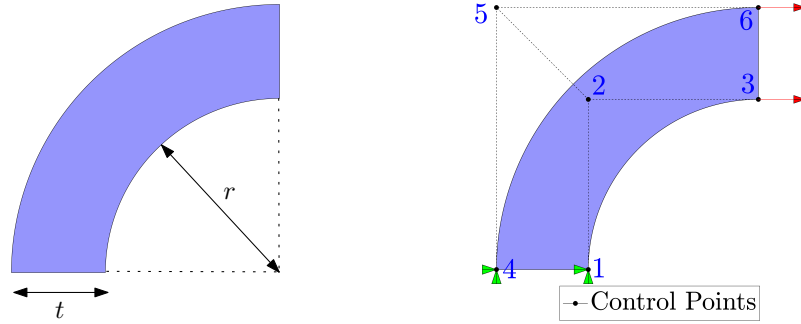


Figure 4: Uncertain geometric parameters of the quarter-circular annulus (left) and isogeometric model with boundary conditions (right).

718 The geometry is represented using $n_{cp} = 6$ control points. The corresponding NURBS control-
 719 point matrix $\mathbf{P}$ is parameterized in terms of the uncertain radius r and thickness t as

$$\mathbf{P} = \begin{bmatrix} t & t & t+r & 0 & 0 & t+r \\ 0 & r & r & 0 & t+r & t+r \end{bmatrix}^T. \quad (56)$$

720 Additional implementation details of the IGA model are provided in Appendix B.

721 A high-fidelity database of 10000 Latin Hypercube Sampling realizations was partitioned into
 722 a training pool of 9000 samples and a fixed validation set of 1000 samples. For each training size,
 723 an independent random subset of n_{sim} simulations was generated without replacement from the
 724 training pool, with n_{sim} ranging up to 200. Each selected location provides the response and the

725 corresponding geometry-consistent sensitivity vector. The validation responses and sensitivities
 726 were used exclusively for out-of-sample assessment and were not involved in surrogate fitting or
 727 model selection.

728 The candidate maximum polynomial orders were $p_p \in \{6, 7, 8\}$ for all numerical examples,
 729 as determined from preliminary evaluations over a broader range of polynomial orders. Lower-
 730 order expansions showed insufficient approximation capacity for the response surfaces considered,
 731 whereas orders beyond $p_p = 8$ produced only marginal improvements in predictive accuracy,
 732 indicating that the approximation error had begun to plateau. This range was therefore retained
 733 as a common candidate set, with the polynomial order selected independently for each surrogate
 734 and training realization according to the corresponding model-selection criterion. For the response-
 735 only sparse polynomial chaos expansion based on least-angle regression (PCE-LAR), the order
 736 was selected using the analytical response leave-one-out error [21]. For the proposed IGA-based
 737 sensitivity-enhanced polynomial chaos expansion (IGA-SE PCE), the order was selected using a
 738 grouped leave-one-simulation-out score that equally combines the variance-normalized response
 739 and sensitivity errors. For its sparse least-angle-regression variant (IGA-SE PCE-LAR), the
 740 grouped criterion was based on the held-out response error evaluated on the selected active basis.
 741 In both grouped procedures, the response equation and the two sensitivity equations associated
 742 with the held-out simulation were removed simultaneously. Derivative accuracy was subsequently
 743 evaluated on the fixed validation set against the corresponding IGA variational sensitivities.

744 Figure 5 compares the predictive accuracy of PCE-LAR (blue), IGA-SE PCE (red), IGA-
 745 SE PCE-LAR (green), and gradient-enhanced Kriging using central finite-difference sensitivities
 746 (GEK-FD, black). GEK-FD provides an external derivative-informed benchmark in which gra-
 747 dient observations are obtained through additional high-fidelity evaluations using central finite
 748 differences. A squared-exponential covariance kernel with separate length scales is employed,
 749 with hyperparameters re-estimated by maximum likelihood for each training set and statistical
 750 repetition. Further implementation and optimization details are provided in Appendix C. The
 751 comparison with GEK-FD is interpreted as a cost-consistent comparison of complete surrogate-
 752 construction workflows rather than as evidence of intrinsic superiority of either surrogate family.

753 Three response-error metrics are considered: the mean squared error (MSE), the cumulative
 754 absolute error, and the maximum absolute error. All results are based on 50 independent repe-
 755 titions, and the convergence curves report the mean together with ± 1 standard-deviation bands.

For the MSE panel, these statistics are computed after applying the base-10 logarithm to the MSE obtained in each repetition. The horizontal axis represents the equivalent high-fidelity computational effort, including the additional cost of sensitivity acquisition as detailed in Section 6.5.

Across the three response metrics, the sensitivity-enhanced PCE formulations improve upon the response-only PCE-LAR baseline, particularly in the low-cost regime. IGA-SE PCE attains the lowest mean squared and cumulative absolute errors over much of the low- and intermediate-cost range, while GEK-FD becomes increasingly competitive at larger computational budgets and provides particularly low maximum errors over part of the investigated range. The overlap of the standard-deviation bands further indicates that the relative performance depends on the selected experimental design. Table 1 complements these trends and shows that IGA-SE PCE reaches both prescribed mean MSE levels with the lowest equivalent computational effort among the compared methods.

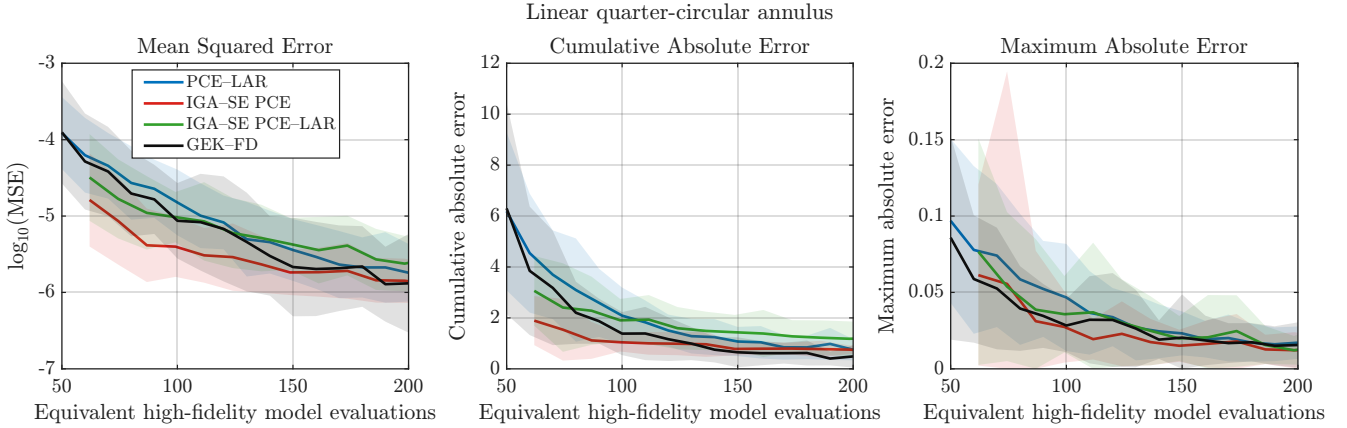


Figure 5: Comparison of surrogate-model accuracy for the maximum stress triaxiality in the linear quarter-circular annulus over a common range of up to 200 equivalent high-fidelity model evaluations. Solid lines denote the mean performance over the statistical repetitions, and the shaded regions represent one standard deviation.

The response comparison is complemented by the out-of-sample derivative assessment in Figure 6. The first two panels report the mean squared errors of the derivatives with respect to r and t , while the third reports the combined normalized gradient error obtained by summing the component-wise MSEs normalized by the corresponding validation-set gradient variances. IGA-SE PCE consistently improves the out-of-sample derivative predictions relative to the response-only PCE-LAR baseline. IGA-SE PCE-LAR also reduces the gradient errors over most of the common cost range, while GEK-FD remains competitive at intermediate and high computational budgets. Together, the response and derivative results show that the IGA-derived sensitivities improve both response and gradient approximation, with the clearest response gains occurring in the low-cost

Table 1: Equivalent computational effort required by the surrogate models to achieve prescribed mean squared error levels for the linear quarter-circular annulus. The equivalent number of high-fidelity (HF) evaluations accounts for the additional cost associated with sensitivity computations. Non-integer equivalent costs are conservatively rounded up to the next integer high-fidelity evaluation.

Method	ϵ_{target}	Equivalent HF evaluations	Achieved mean MSE
PCE-LAR	10^{-4}	70	7.43×10^{-5}
	10^{-5}	130	8.67×10^{-6}
IGA-SE PCE	10^{-4}	62	4.93×10^{-5}
	10^{-5}	100	6.43×10^{-6}
IGA-SE PCE-LAR	10^{-4}	62	7.96×10^{-5}
	10^{-5}	137	8.96×10^{-6}
GEK-FD	10^{-4}	80	4.13×10^{-5}
	10^{-5}	140	6.33×10^{-6}

777 regime.

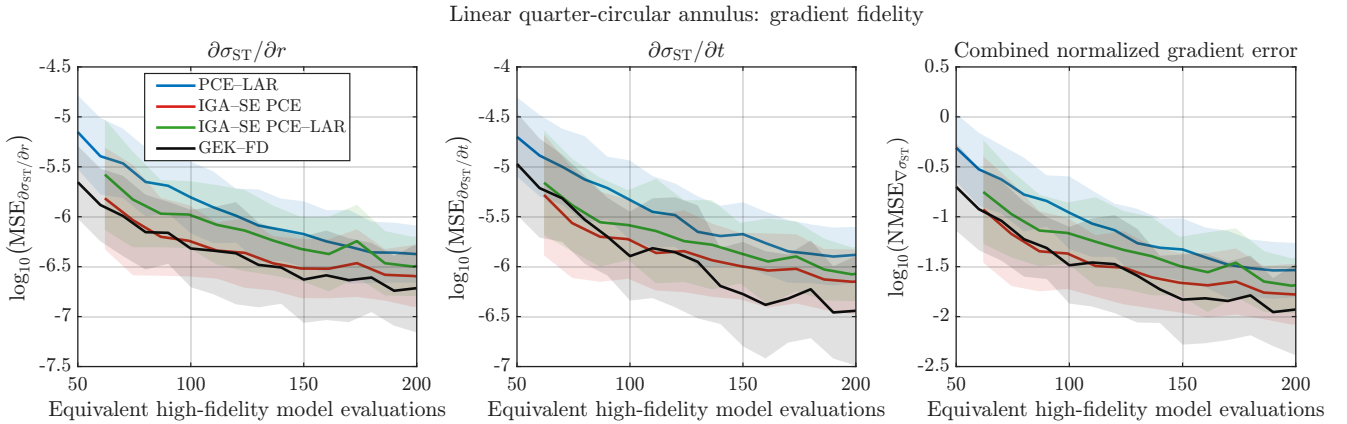
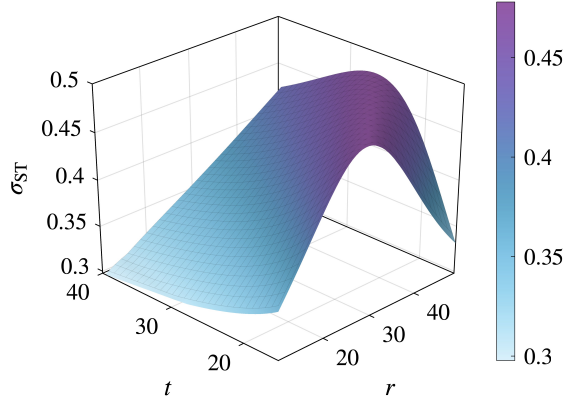
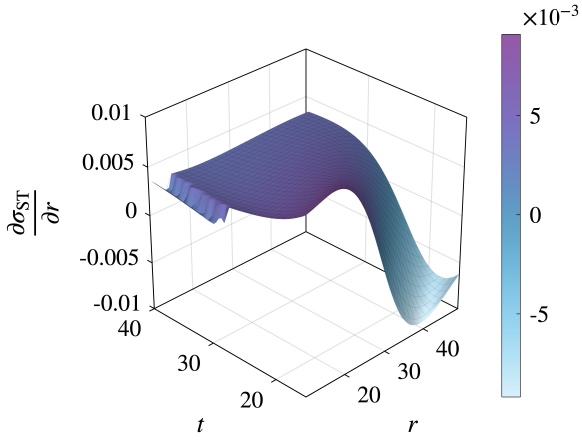


Figure 6: Comparison of out-of-sample derivative accuracy for the linear quarter-circular annulus over a common range of up to 200 equivalent high-fidelity model evaluations. Derivatives are evaluated against the held-out IGA variational sensitivities. Solid lines denote the mean performance over the statistical repetitions, and the shaded regions represent one standard deviation.

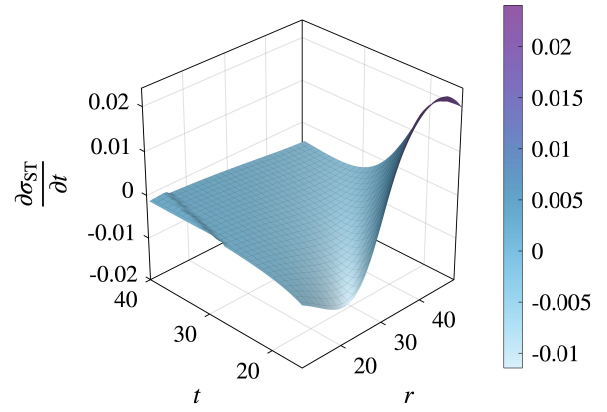
778 Figure 7 provides a complementary view of the geometry-dependent response and sensitivity
779 fields. The stress-triaxiality surface $\sigma_{ST}(r, t)$ exhibits pronounced curvature and non-monotonic
780 behavior over the admissible parameter domain. The corresponding sensitivity fields show different
781 directional effects, with variations in r producing relatively smooth changes and variations in t
782 producing more localized regions of elevated sensitivity. These patterns illustrate the need to
783 reproduce both response values and geometry-dependent sensitivity trends over the uncertain
784 parameter space. Selected spatial stress-triaxiality distributions are provided in Appendix B.1 in
785 Figure B.15. They further illustrate the redistribution of the stress field induced by variations in
786 r and t .



(a) Stress triaxiality surface $\sigma_{ST}(r, t)$.



(b) Sensitivity $\partial\sigma_{ST}/\partial r$.



(c) Sensitivity $\partial\sigma_{ST}/\partial t$.

Figure 7: IGA maximum stress-triaxiality response and sensitivity surfaces for the quarter-circular annulus as functions of the radius r and thickness t .

6.2. Solid horseshoe

This example assesses the ability of the proposed IGA-based sensitivity-enhanced PCE formulation to approximate geometry-dependent stress-triaxiality variations in a three-dimensional setting involving four uncertain geometric parameters. The framework is applied to a three-dimensional horseshoe-shaped solid adapted from Hughes [10], shown in Figure 8. The structure is subjected to equal and opposite prescribed displacements $\pm u_0$ along the flat edges in the x -direction. Additional displacement constraints are imposed to prevent rigid-body motions. These include supports at the base ends in the y -direction and localized constraints at the outer corners and top region of the horseshoe. The constrained control-point degrees of freedom are indicated by the green markers in Figure 8. The material behavior is assumed deterministic and linear elastic, with Young's modulus $E = 3 \times 10^7 \text{ N/cm}^2$ and Poisson's ratio $\nu = 0.3$.

The horseshoe geometry is constructed through a U-sweep of a square cross-section of dimen-

799 sions $L \times L$. A quarter disk of radius R is removed to define the inner edge. The geometry also
 800 includes a straight segment of height H , while r controls the position of the inner circular region
 801 relative to the origin. The resulting NURBS volume contains $n_{cp} = 108$ control points, corre-
 802 sponding to 324 geometric degrees of freedom. The control-point coordinates are parameterized
 803 directly in terms of the uncertain geometric parameters (L, R, r, H) . Additional implementation
 804 details of the parameterization and design-velocity matrix are provided in Appendix D. The pa-
 805 rameters are modeled as independent uniform random variables: $L \sim \mathcal{U}(3.5, 5.5)$, $R \sim \mathcal{U}(0.5, 1.5)$,
 806 $r \sim \mathcal{U}(0.9142, 1.9142)$, and $H \sim \mathcal{U}(7.5, 8.5)$, with all quantities expressed in cm.

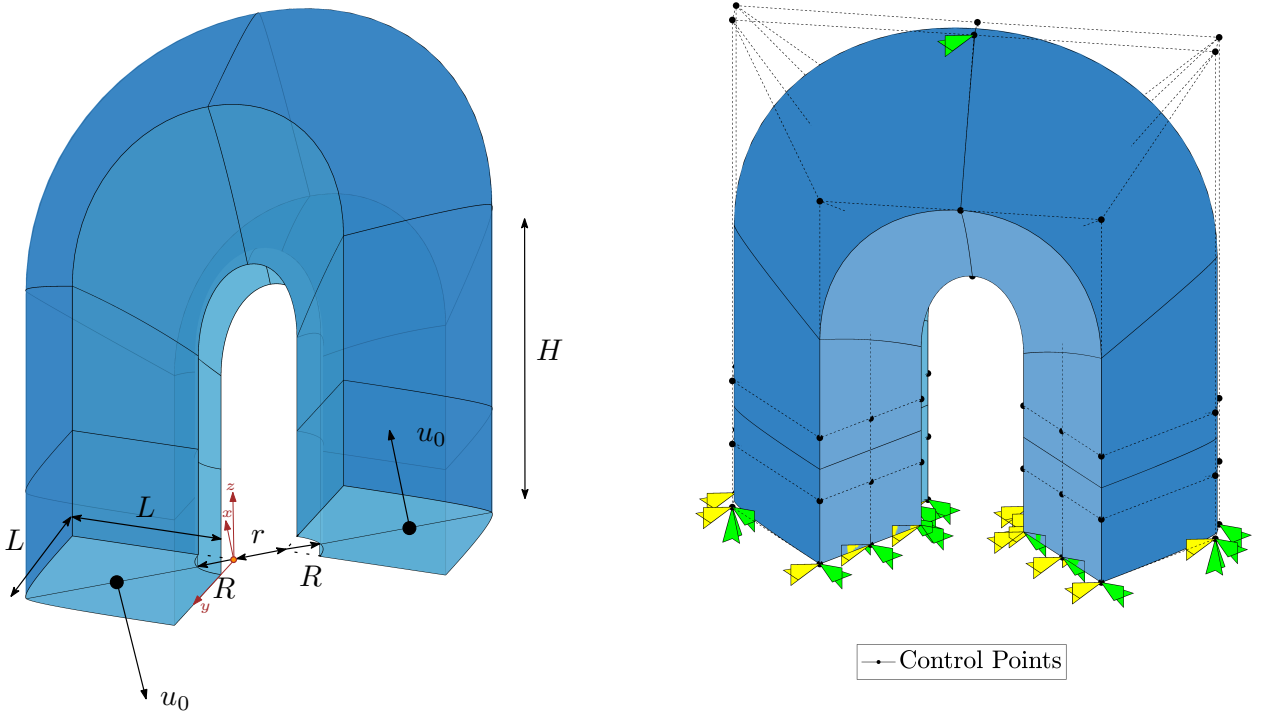


Figure 8: Geometry and boundary conditions of the three-dimensional horseshoe example. The left panel shows the uncertain geometric parameters and prescribed flat-edge displacements, while the right panel shows the corresponding isogeometric model with NURBS control points and boundary conditions. Yellow markers indicate non-zero prescribed displacements ($u_x = \pm u_0$), green markers indicate homogeneous displacement constraints, and black dots denote the NURBS control points.

807 The main NURBS and discretization settings are summarized in Table 2. The complete para-
 808 metric definition of the control net is provided in Appendix D.

809 The training and validation protocol follows Section 6.1. A database of 10000 Latin Hypercube
 810 Sampling realizations is partitioned into a training pool of 9000 samples and a fixed validation set
 811 of 1000 samples. Experimental designs are selected without replacement from the training pool,
 812 and all reported curves are obtained from 50 independent designs. The candidate polynomial-
 813 degree range is again $p_p \in \{6, 7, 8\}$. For PCE-LAR, the degree is selected using the analytical

Table 2: NURBS and discretization settings for the three-dimensional horseshoe example.

Quantity	Value
Parametric directions	(ξ, η, ζ)
Polynomial degrees	$(p, q, r) = (2, 2, 2)$
Number of basis functions	$(n_\xi, n_\eta, n_\zeta) = (4, 3, 9)$
Number of control points	$n_{\text{cp}} = 4 \times 3 \times 9 = 108$
Degrees of freedom	$3n_{\text{cp}} = 324$
Number of knot spans/elements	$2 \times 1 \times 6 = 12$
Design-velocity matrix size	$\mathbf{D} \in \mathbb{R}^{324 \times 4}$

814 response leave-one-out error. For IGA–SE PCE, the grouped criterion combines the variance-
815 normalized response error and the four sensitivity errors. For IGA–SE PCE–LAR, the grouped
816 criterion uses the held-out response error on the active basis. In both grouped procedures, the
817 response and all four sensitivity equations associated with the held-out realization are removed
818 simultaneously. The model-selection criteria use only the training data. The sensitivity overhead
819 is included in the equivalent computational cost and is quantified in Section 6.5.

820 Figure 9 compares the response accuracy of the four surrogate models as a function of the
821 equivalent high-fidelity computational cost. The sensitivity-enhanced PCE formulations become
822 increasingly competitive with PCE–LAR as the available computational budget increases. Beyond
823 approximately 200 equivalent high-fidelity evaluations, they generally achieve comparable or lower
824 mean squared errors and lower cumulative absolute errors over much of the investigated range.
825 The maximum absolute error shows a different trend, with PCE–LAR providing the smallest
826 maximum validation error. Thus, the additional derivative information primarily improves global
827 approximation quality rather than uniformly reducing the largest local errors.

828 GEK–FD generally exhibits larger mean squared and cumulative response errors in this bench-
829 mark. The additional high-fidelity evaluations required for finite-difference gradients reduce the
830 number of training locations available at a given equivalent computational budget. The full
831 and sparse IGA–SE formulations show broadly similar convergence trends. However, IGA–SE
832 PCE–LAR reaches the stricter response-accuracy target at a lower equivalent cost than the full
833 sensitivity-enhanced formulation. Table 3 confirms that all methods reach the 10^{-3} target at
834 comparable costs, whereas IGA–SE PCE–LAR reaches the 10^{-4} target with the lowest equivalent
835 computational effort. GEK–FD does not reach the latter target within the investigated range.

836 Figure 10 compares the out-of-sample accuracy of the four geometry-dependent derivatives.
837 The effect of sensitivity enrichment is clearly direction-dependent. For the derivatives with respect

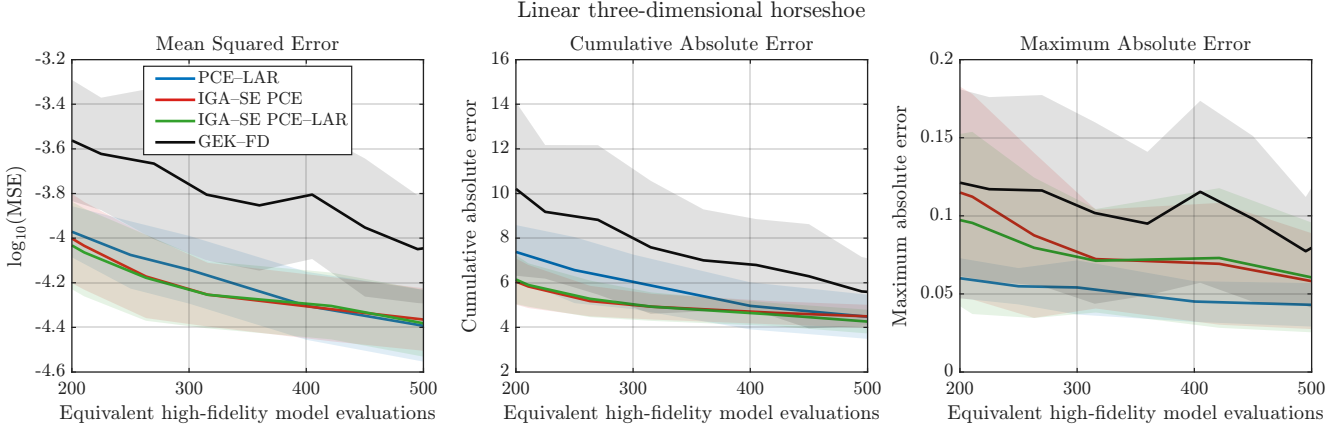


Figure 9: Comparison of response accuracy for the maximum stress triaxiality of the three-dimensional horseshoe over a common range of up to 500 equivalent high-fidelity response evaluations. Solid lines show mean values over 50 independent experimental designs, and shaded regions show one standard deviation.

Table 3: Equivalent computational effort required by the surrogate models to achieve prescribed mean squared error levels for the three-dimensional linear horseshoe benchmark. The equivalent number of high-fidelity (HF) evaluations accounts for the additional computational cost associated with variational sensitivity evaluations in the IGA-SE models and finite-difference gradient evaluations in GEK-FD. Non-integer equivalent costs are conservatively rounded up to the next high-fidelity evaluation.

Method	ϵ_{target}	Equivalent HF evaluations	Achieved mean MSE
PCE-LAR	10^{-3}	125	1.81×10^{-4}
	10^{-4}	250	9.01×10^{-5}
IGA-SE PCE	10^{-3}	132	2.56×10^{-4}
	10^{-4}	264	7.42×10^{-5}
IGA-SE PCE-LAR	10^{-3}	132	1.75×10^{-4}
	10^{-4}	211	9.65×10^{-5}
GEK-FD	10^{-3}	135	4.52×10^{-4}
	10^{-4}	—	—

to R and r , both IGA-SE PCE formulations generally provide the lowest errors over most of the investigated cost range. For the derivative with respect to L , the differences between the polynomial-chaos models are smaller, with PCE-LAR reaching slightly lower errors toward the upper end of the range. For the derivative with respect to H , GEK-FD provides the smallest error.

This behavior is consistent with the relative influence of the geometric parameters. The maximum stress triaxiality is considerably more sensitive to variations in R than in H , while the influence of H is comparatively small. The raw combined gradient error generally favors the sensitivity-enhanced formulations over much of the investigated range. After variance normalization, the differences between the methods become smaller. This indicates that the benefit of

Linear three-dimensional horseshoe: gradient fidelity

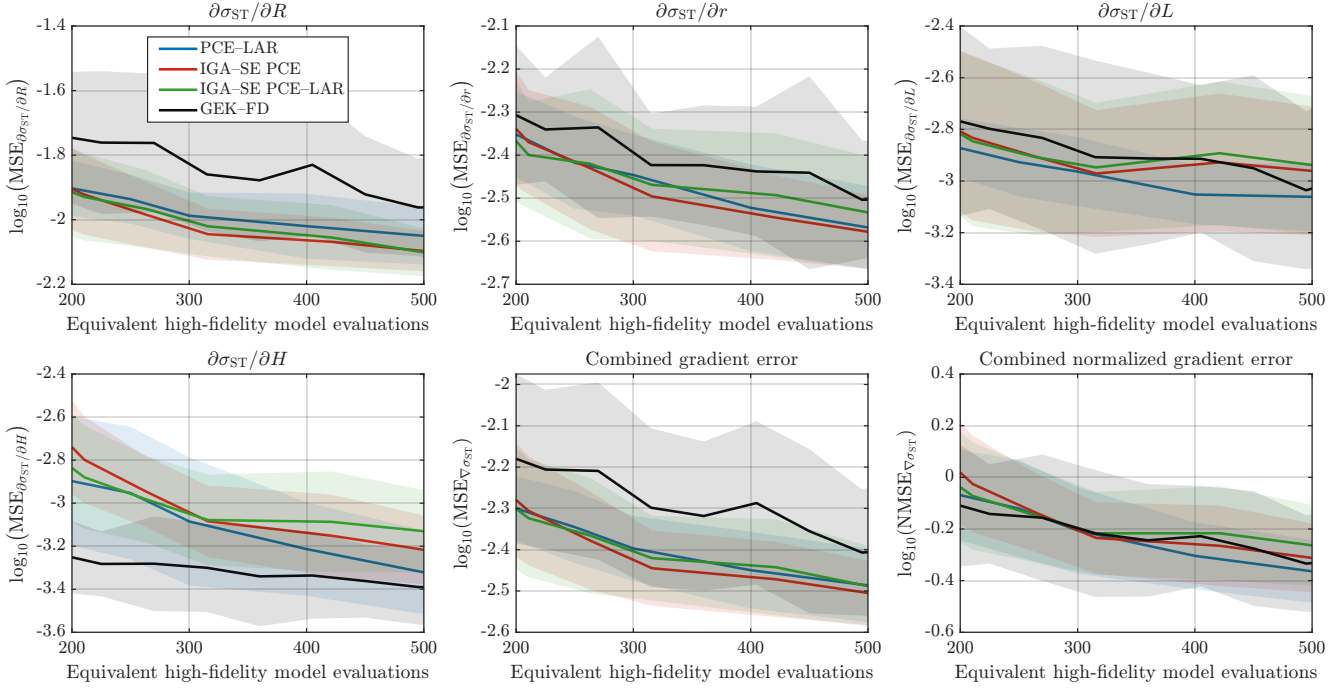


Figure 10: Comparison of out-of-sample derivative accuracy for the maximum stress triaxiality of the three-dimensional horseshoe. The first four panels report the component-wise derivative MSEs, while the last two panels report the combined and variance-normalized gradient errors.

sensitivity enrichment is not distributed uniformly across the individual geometric directions and is more pronounced for some of the dominant sensitivities.

Selected spatial stress-triaxiality distributions are provided in Appendix D.1 (Figure D.16). They further illustrate how geometric variability modifies the localization, intensity, and spatial extent of the stress-triaxiality field.

6.3. Nonlinear quarter-circular annulus

The objective of this example is to assess the applicability of the proposed framework beyond linear elasticity by revisiting the quarter-circular annulus of Section 6.1 using a nonlinear isogeometric formulation. The same geometry, uncertain parameters, boundary conditions, and response quantity are retained. Thus, the inner radius r and thickness t are again modeled as independent uniform random variables, with $r \sim \mathcal{U}(10, 50)$ mm and $t \sim \mathcal{U}(15, 40)$ mm. This configuration assesses the nonlinear formulation within the same geometric uncertainty setting as the linear benchmark.

The benchmark is analyzed using a compressible Neo-Hookean material model under plane-strain conditions. Young's modulus, Poisson's ratio, and the out-of-plane thickness are fixed at

863 $E = 2 \times 10^5 \text{ N/mm}^2$, $\nu = 0.3$, and 1 mm, respectively. The response is computed incrementally
864 using 10 equal load steps. At each step, the nonlinear equilibrium problem is solved using the
865 Newton–Raphson procedure described in Section 4.2.2, with a residual tolerance of 10^{-8} and a
866 maximum of 25 iterations. After convergence of the final load step, the variational sensitivity
867 problem is solved using the converged tangent stiffness matrix and the geometry-induced pseudo-
868 load terms described in Section 4.3. The resulting displacement sensitivities are propagated during
869 post-processing to obtain sensitivities of the stress-based quantities of interest.

870 The nonlinear variational sensitivities were verified against central finite-difference approxi-
871 mations using a perturbation size of $h = 10^{-4}$ over the 10000 realizations. The median relative
872 discrepancies were 1.17×10^{-8} for $\partial\sigma_{5T}/\partial r$ and 1.11×10^{-8} for $\partial\sigma_{5T}/\partial t$. The corresponding
873 99th percentiles were 1.09×10^{-6} and 1.05×10^{-6} , respectively. The selected loading produces
874 moderate finite-deformation levels. At the nominal geometry, the maximum absolute principal
875 Green–Lagrange strain reaches 4.61×10^{-2} . Under otherwise identical plane-strain conditions,
876 the Neo-Hookean displacement vector differs from its small-strain linear counterpart by 6.64% in
877 relative Euclidean norm. Across representative realizations spanning the uncertainty domain, this
878 difference ranges from 1.28% to 25.34%. These results confirm that the benchmark includes both
879 nearly linear and appreciably nonlinear response regimes.

880 The response of interest remains the maximum stress triaxiality σ_{5T} , computed from the
881 Cauchy stress tensor according to Eq. (55). For each selected realization, the nonlinear IGA
882 model provides the response and the variational sensitivities with respect to r and t . The physi-
883 cal sensitivities are transformed to the standardized stochastic space according to Eq. (54). The
884 database, training–validation partition, experimental-design generation, polynomial-order selec-
885 tion, and statistical assessment follow the protocol introduced in Section 6.1. Derivative accuracy
886 is evaluated independently on the fixed validation set using the corresponding IGA variational
887 sensitivities.

888 Figure 11 compares the response accuracy of PCE–LAR, IGA–SE PCE, IGA–SE PCE–LAR,
889 and GEK–FD over a common range of up to 200 equivalent high-fidelity evaluations. The same
890 response-error metrics and equivalent-cost definition introduced for the linear benchmark are em-
891 ployed. Additional implementation and optimization details for GEK–FD are provided in Ap-
892 pendix C.

893 Across the three response metrics, IGA–SE PCE provides the lowest or nearly lowest mean error

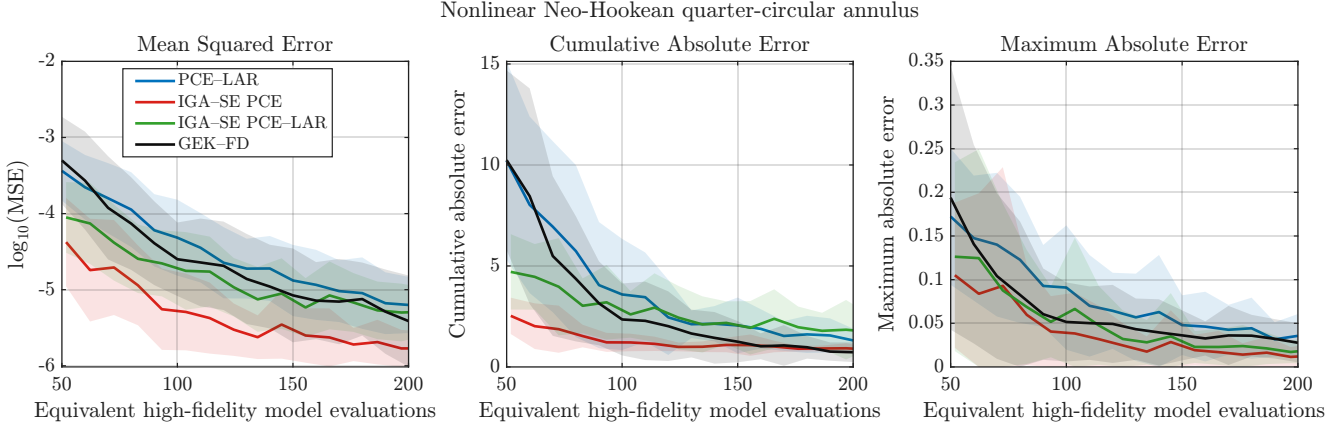


Figure 11: Comparison of surrogate-model accuracy for the maximum stress triaxiality in the nonlinear Neo-Hookean quarter-circular annulus over a common range of up to 200 equivalent high-fidelity model evaluations. Solid lines denote the mean performance over the 50 statistical repetitions, and the shaded regions represent one standard deviation.

over most of the common cost range, with the clearest advantage in the low-data regime. IGA-SE PCE-LAR also improves upon the response-only baseline over most of the investigated range, while GEK-FD becomes increasingly competitive as the computational budget increases. The overlap of the variability bands indicates that the relative performance depends on the selected experimental design and should therefore be interpreted through the overall statistical trends rather than strict dominance. Table 4 shows that IGA-SE PCE reaches both prescribed mean MSE levels with the lowest equivalent computational effort. For the more restrictive threshold of 10^{-5} , it reduces the required effort by approximately 43% relative to both PCE-LAR and GEK-FD. All four methods nevertheless reach both reported accuracy levels within the investigated range.

Table 4: Equivalent computational effort required by the surrogate models to achieve prescribed mean squared error levels for the nonlinear quarter-circular annulus. The equivalent number of high-fidelity (HF) evaluations accounts for the additional cost associated with sensitivity computations. Non-integer equivalent costs are conservatively rounded up to the next high-fidelity evaluation.

Method	ϵ_{target}	Equivalent HF evaluations	Achieved mean MSE
PCE-LAR	10^{-4}	100	9.88×10^{-5}
	10^{-5}	200	9.55×10^{-6}
IGA-SE PCE	10^{-4}	52	9.89×10^{-5}
	10^{-5}	115	9.15×10^{-6}
IGA-SE PCE-LAR	10^{-4}	83	4.60×10^{-5}
	10^{-5}	156	9.86×10^{-6}
GEK-FD	10^{-4}	100	7.06×10^{-5}
	10^{-5}	200	9.77×10^{-6}

Figure 12 complements the response comparison with the out-of-sample derivative accuracy. The first two panels report the errors in $\partial\sigma_{\text{ST}}/\partial r$ and $\partial\sigma_{\text{ST}}/\partial t$, while the third reports the combined normalized gradient error. IGA-SE PCE provides the lowest mean combined gradient error throughout the common cost range, with the same general trend observed for both individual derivative components. IGA-SE PCE-LAR and GEK-FD remain competitive as the computational budget increases. Together with the response results, these findings show that the variational sensitivities improve both response and derivative approximation for the nonlinear benchmark.

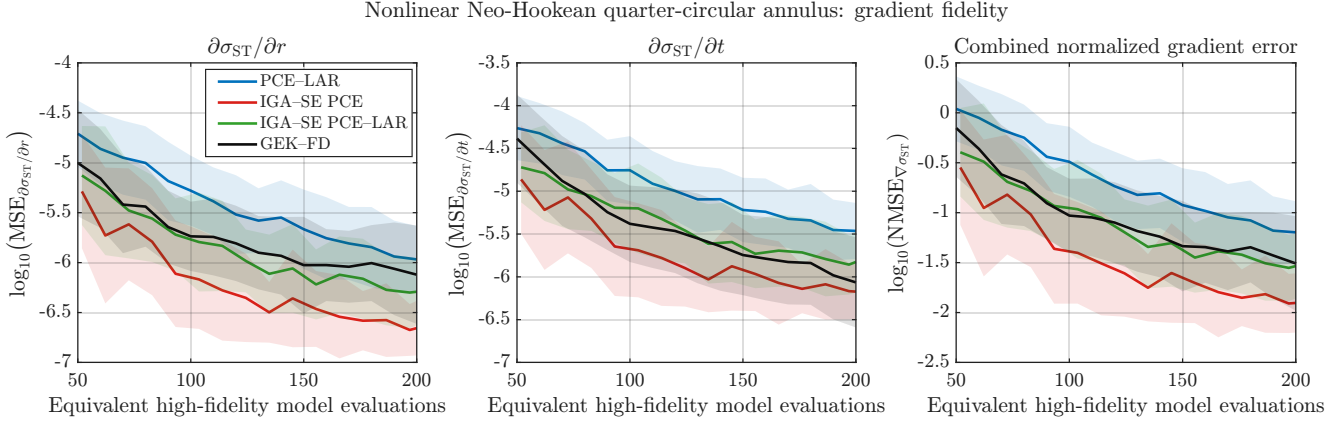


Figure 12: Comparison of out-of-sample derivative accuracy for the nonlinear Neo-Hookean quarter-circular annulus over a common range of up to 200 equivalent high-fidelity model evaluations. Derivatives are evaluated against the held-out IGA variational sensitivities. The combined normalized gradient error is obtained by summing the component-wise mean squared errors normalized by the corresponding validation-set gradient variances. Solid lines denote the mean performance over the 50 statistical repetitions, and the shaded regions represent one standard deviation.

6.4. Quarter-circular annulus with combined geometric and material uncertainty

The final example assesses whether geometry-derived variational sensitivities remain beneficial when the structural response is also influenced by an independent uncertain material parameter. The nonlinear quarter-circular annulus of Section 6.3 is therefore extended by introducing uncertainty in Poisson's ratio while retaining the same geometry, boundary conditions, loading, and quantity of interest. The geometric parameters remain independent uniform random variables, with $r \sim \mathcal{U}(10, 50)$ mm and $t \sim \mathcal{U}(15, 40)$ mm. Young's modulus and the out-of-plane thickness remain fixed at $E = 2 \times 10^5$ N/mm² and 1 mm, respectively. Poisson's ratio is modeled according to

$$Z_\nu \sim \text{Beta}(\alpha_\nu, \beta_\nu), \quad \nu = 0.5Z_\nu, \quad (\alpha_\nu, \beta_\nu) = (39.4, 26.2667), \quad (57)$$

which yields $\mu_\nu = 0.3$ and a coefficient of variation $\text{CoV}_\nu = 0.1$. The PCE is therefore constructed in three independent stochastic dimensions associated with (r, t, ν) . The geometric variables are

transformed according to Eq. (53), while ν is represented through $U_\nu \sim \mathcal{U}(0,1)$ and mapped to its physical value using the inverse beta cumulative distribution function.

The compressible Neo-Hookean formulation, plane-strain assumption, and nonlinear solution strategy are unchanged from the previous benchmark. Derivative information, however, remains available only with respect to the geometric parameters r and t . Consequently, the polynomial basis spans the full three-dimensional stochastic space, whereas derivative information is incorporated only along two stochastic directions. This increases the approximation complexity while providing no derivative enrichment for the uncertain material parameter.

The database generation, training-validation partition, polynomial-order selection, and statistical assessment follow the protocol of Section 6.3. The database is generated in the three-dimensional uncertain space associated with (r, t, ν) . GEK-FD is constructed in the corresponding physical parameter space and uses central finite-difference derivatives only with respect to r and t . Additional implementation and optimization details are provided in Appendix C.

Figure 13 compares the response accuracy of PCE-LAR, IGA-SE PCE, IGA-SE PCE-LAR, and GEK-FD over a common range of up to 600 equivalent high-fidelity evaluations. The same response-error metrics and statistical summaries introduced in the preceding benchmarks are employed.

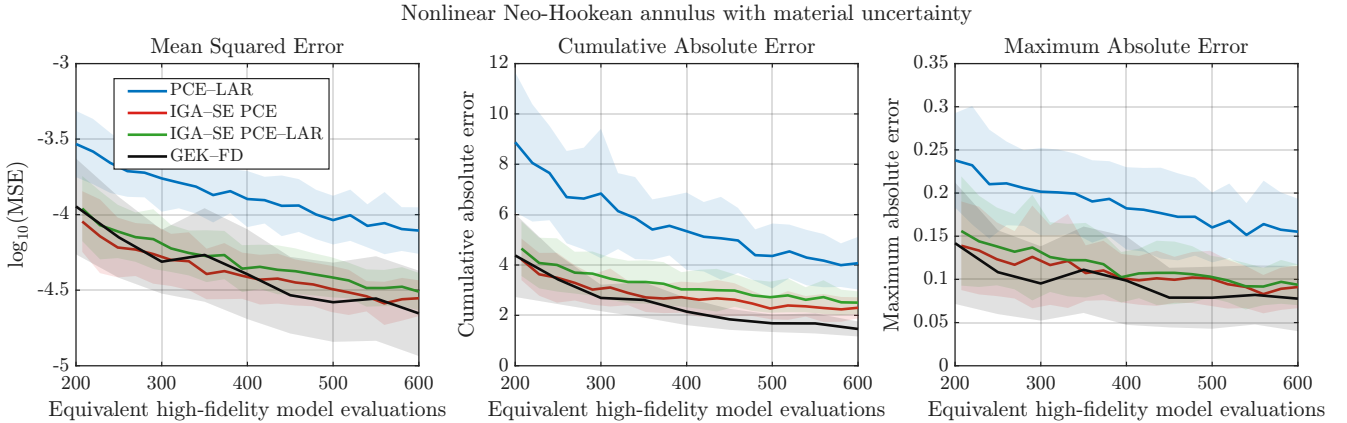


Figure 13: Comparison of surrogate-model accuracy for the maximum stress triaxiality in the nonlinear Neo-Hookean quarter-circular annulus with combined geometric and material uncertainty over a common range of up to 600 equivalent high-fidelity model evaluations. Solid lines denote the mean performance over the 50 statistical repetitions, and the shaded regions represent one standard deviation.

Both sensitivity-enhanced PCE formulations improve upon PCE-LAR over the common cost range, with the largest gains occurring in the low-data regime. At the lowest investigated budget, IGA-SE PCE reduces the mean MSE by approximately 70% relative to PCE-LAR and by

approximately 40% relative to GEK–FD. As the computational budget increases, GEK–FD becomes increasingly competitive and provides the lowest mean response errors near the upper end of the investigated range. The sensitivity-enhanced formulations nevertheless retain lower mean response errors than PCE–LAR over the investigated range. The overlap of the variability bands indicates that the relative ordering also depends on the selected experimental design.

Table 5 summarizes the equivalent computational effort required to reach the prescribed mean MSE levels. Both sensitivity-enhanced formulations reach the 10^{-4} threshold at lower equivalent cost than GEK–FD and substantially lower cost than PCE–LAR. For the stricter threshold of 5×10^{-5} , IGA–SE PCE requires the lowest equivalent computational effort, whereas PCE–LAR does not reach this accuracy within the investigated range.

Table 5: Equivalent computational effort required by the surrogate models to achieve prescribed mean squared error levels for the nonlinear quarter-circular annulus with combined geometric and material uncertainty. The equivalent number of high-fidelity (HF) evaluations accounts for the additional cost associated with sensitivity computations. Non-integer equivalent costs are conservatively rounded up to the next high-fidelity evaluation.

Method	ϵ_{target}	Equivalent HF evaluations	Achieved mean MSE
PCE–LAR	10^{-3}	200	3.33×10^{-4}
	10^{-4}	500	9.88×10^{-5}
	5×10^{-5}	—	—
IGA–SE PCE	10^{-3}	208	1.01×10^{-4}
	10^{-4}	229	8.48×10^{-5}
	5×10^{-5}	353	4.39×10^{-5}
IGA–SE PCE–LAR	10^{-3}	208	1.26×10^{-4}
	10^{-4}	229	9.81×10^{-5}
	5×10^{-5}	394	4.69×10^{-5}
GEK–FD	10^{-3}	200	1.66×10^{-4}
	10^{-4}	250	8.77×10^{-5}
	5×10^{-5}	450	3.54×10^{-5}

Figure 14 complements the response comparison with the out-of-sample derivative accuracy. Both sensitivity-enhanced PCE formulations consistently reduce the derivative errors relative to PCE–LAR over the common cost range. GEK–FD provides a similarly accurate derivative-informed benchmark, and the combined normalized gradient errors of the three derivative-enhanced approaches become nearly identical near the upper end of the range. The individual derivative components nevertheless show complementary behavior. The IGA–SE formulations provide lower errors for the radial derivative, whereas GEK–FD becomes more accurate for the thickness derivative at the largest computational budgets.

960 Compared with the geometry-only nonlinear benchmark, the performance differences between
 961 the derivative-enhanced approaches are smaller. This reflects the additional uncertainty in ν , for
 962 which no derivative information is incorporated during surrogate construction. Nevertheless, the
 963 results show that geometry-derived variational sensitivities remain informative when derivative
 964 enrichment is available only along a subset of the stochastic directions.

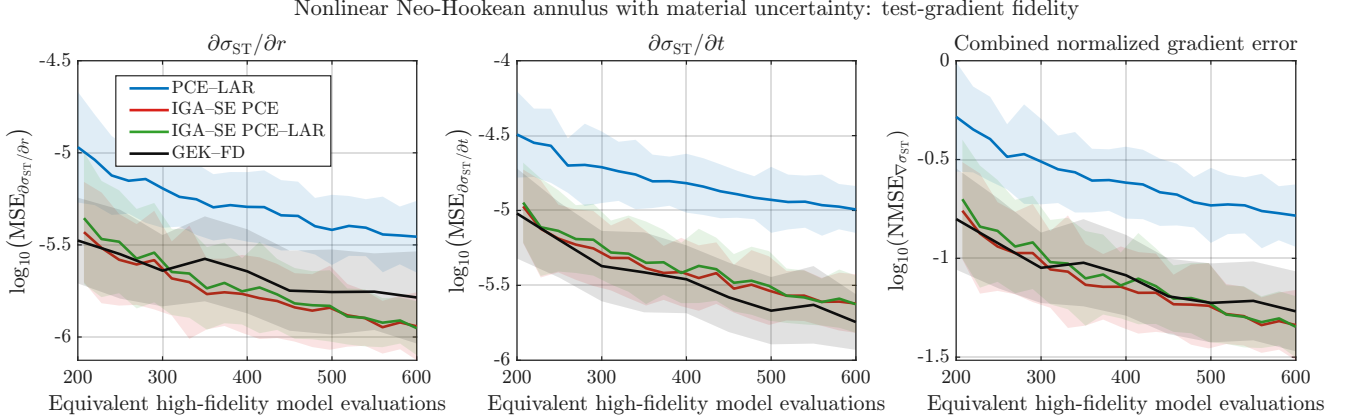


Figure 14: Comparison of out-of-sample derivative accuracy for the nonlinear Neo-Hookean quarter-circular annulus with combined geometric and material uncertainty over a common range of up to 600 equivalent high-fidelity model evaluations. Derivatives are evaluated against the held-out IGA variational sensitivities. The combined normalized gradient error is obtained by summing the component-wise mean squared errors normalized by the corresponding validation-set gradient variances. Solid lines denote the mean performance over the 50 statistical repetitions, and the shaded regions represent one standard deviation.

965 6.5. Computational cost and interpretation of the sensitivity enrichment

966 The previous examples show that incorporating IGA-derived variational sensitivities improves
 967 the accuracy of the PCE surrogate compared with the corresponding response-only sparse PCE
 968 baseline. This improvement is obtained by enriching each training realization with derivative
 969 information, and therefore the additional cost of computing these sensitivities must be considered.

970 In the proposed formulation, each training point requires one high-fidelity IGA response evalu-
 971 ation and the solution of the associated variational sensitivity problem. For comparison, obtaining
 972 gradient information with the same number of geometric derivative components through finite dif-
 973 ferences would require additional high-fidelity response evaluations at each training point. Let M
 974 denote the number of geometric directions for which derivative information is supplied. Forward
 975 finite differences then require $M + 1$ high-fidelity analyses per training point, while central finite
 976 differences require $2M + 1$ analyses. In contrast, the proposed variational approach requires one
 977 primal IGA solve plus the additional sensitivity overhead. This cost structure is summarized in
 978 Table 6.

Table 6: Relative computational cost of different strategies for obtaining response and gradient information at one training point. The relative costs are expressed with respect to one high-fidelity response evaluation.

Strategy	Computational requirement per training point	Relative cost
Response-only IGA evaluation	1	1
IGA response + variational sensitivities	1 primal solve + sensitivity overhead	$1 + \eta_{\text{sens}}$
Forward finite-difference gradients	$M + 1$	$M + 1$
Central finite-difference gradients	$2M + 1$	$2M + 1$

Here, η_{sens} denotes the measured relative overhead of the variational sensitivity evaluation with respect to one response-only IGA analysis. The relative sensitivity overhead η_{sens} was quantified from repeated MATLAB executions of the response-only and response-plus-sensitivity analyses. Median runtimes were used to define the equivalent-cost factors reported in Table 7.

Table 7: Measured computational overhead of the variational sensitivity analysis for the two-dimensional annulus benchmarks. Times correspond to median runtimes over 1000 repeated evaluations in MATLAB.

Case	Response-only [s]	Response + sensitivities [s]	η_{sens}
Linear elasticity	3.17×10^{-3}	3.93×10^{-3}	23.96%
Neo-Hookean	5.50×10^{-2}	5.70×10^{-2}	3.64%

For the linear elastic annulus, the measured overhead is 23.96%, whereas the nonlinear Neo-Hookean benchmark yields a substantially smaller relative overhead of 3.64%. This reduction does not imply that the sensitivity analysis becomes cheaper. Instead, the nonlinear response evaluation is already dominated by load stepping, Newton iterations, repeated tangent stiffness assemblies, and constitutive updates, so the additional sensitivity computation represents a smaller fraction of the total runtime. The Neo-Hookean factor $1 + \eta_{\text{sens}} = 1.0364$ is therefore used for both nonlinear annulus examples. Although the combined uncertainty benchmark introduces Poisson’s ratio as an additional stochastic variable, the same two geometric sensitivities are computed at every training point. Consequently, the stochastic dimension increases, whereas the gradient-acquisition cost per realization remains unchanged. The same timing procedure was applied to the three-dimensional horseshoe benchmark. The resulting equivalent-cost factor is summarized in Table 8.

Table 8: Measured computational overhead of the variational sensitivity analysis for the three-dimensional horseshoe benchmark. Times correspond to median runtimes over 1000 repeated evaluations in MATLAB.

Case	Response-only [s]	Response + sensitivities [s]	η_{sens}
Linear elasticity	1.1689	1.2308	5.30%

For the three-dimensional horseshoe, the measured overhead is 5.30%, corresponding to an equivalent cost of $n_{\text{eq}} = 1.0530 n_{\text{sim}}$. Since this benchmark supplies sensitivities in four geometric directions ($M = 4$), finite-difference gradients would require five response evaluations with forward differences and nine with central differences at each training point. Compared with the two-dimensional linear example, the relative sensitivity overhead decreases in the three-dimensional benchmark because the primal analysis and full-field post-processing are more demanding. Although sensitivities in four geometric directions are evaluated, quantities from the primal analysis are reused, avoiding the repeated independent high-fidelity analyses required by finite-difference gradient evaluations.

The numerical comparisons reported throughout Section 6 are therefore expressed in terms of equivalent high-fidelity response evaluations. Each training realization of the proposed formulation contributes both the structural response and geometry-consistent sensitivity information. Accordingly, the observed accuracy improvements arise from enriching each training realization with local derivative information obtained consistently within the IGA framework, in addition to the corresponding response value. This represents the central trade-off of the proposed methodology: variational sensitivities incur a moderate additional computational cost, yet they avoid the multiple independent solver calls required by finite-difference gradient evaluations.

The representability of the supplied derivative information was additionally monitored using the relative derivative residual ρ_s defined in Eq. (52). For IGA-SE PCE, the median residuals across all training sizes and repetitions were 5.54%, 19.88%, 2.78%, and 3.51% for the two-dimensional linear, three-dimensional linear, nonlinear, and combined-uncertainty benchmarks, respectively. For IGA-SE PCE-LAR, the corresponding median values were 7.33%, 19.42%, 4.78%, and 3.49%. The larger residuals observed in the three-dimensional benchmark indicate greater incompatibility between the supplied derivative information and the selected finite polynomial spaces, rather than failure of the Moore-Penrose solution. An independent reconstruction of the derivative least-squares problem confirmed that the adopted solution attained the minimum representable derivative residual to numerical precision, with a maximum discrepancy of 9.72×10^{-17} over the reconstructible fits.

7. Conclusions & further work

This paper introduced an IGA-based sensitivity-enhanced polynomial chaos expansion for ge-

ometric uncertainty quantification. The proposed methodology incorporates variational sensitivities computed within an isogeometric analysis model into the PCE regression, using the same NURBS-based representation for geometry parameterization, mechanical analysis, and sensitivity evaluation. The framework was assessed through four linear and nonlinear benchmarks involving low-dimensional geometric uncertainty, including a three-dimensional problem and a case combining geometric and material uncertainty.

Across the investigated benchmarks, sensitivity enrichment generally improved global response prediction and out-of-sample gradient reconstruction relative to the response-only PCE–LAR baseline, with the clearest gains observed in low- and intermediate-cost regimes. The benefit was nevertheless metric- and problem-dependent: improvements were more pronounced for global error measures and dominant sensitivity directions, whereas they were not uniform for maximum-error control or individual gradient components. The results further showed that geometry-derived sensitivities remain informative when derivative information is available only for a subset of the uncertain parameters. The full and sparse sensitivity-enhanced formulations exhibited broadly similar convergence trends, while the sparse formulation provided a favorable cost-to-accuracy trade-off for the stricter response-accuracy target in the three-dimensional benchmark.

Overall, the numerical results indicate that geometry-consistent variational sensitivities can improve the data efficiency of polynomial chaos regression by enriching each high-fidelity realization with local derivative information. The cost-aware assessment showed that these gains can be achieved at a favorable equivalent computational effort for the considered benchmarks, although their magnitude depends on the problem, accuracy measure, and available computational budget. The comparison with GEK–FD further demonstrated competitive performance relative to an external derivative-informed surrogate approach.

The present study is limited to low-dimensional parametric descriptions of admissible NURBS geometries. Moreover, the combined uncertainty example uses geometric sensitivities only and does not include derivatives with respect to material parameters. The external GEK–FD benchmark broadens the comparison beyond the PCE family, but does not establish universal superiority over other gradient-enhanced surrogate models. Accordingly, the reported results should be interpreted as evidence for the considered class of low-dimensional parametric geometric uncertainty problems rather than as a universal assessment of derivative-enhanced surrogate modeling. Furthermore, the extent to which the supplied derivative information can be represented is governed

1055 by the selected finite polynomial space, as quantified by the relative derivative residual.

1056 Future research may extend the proposed formulation to higher-dimensional or localized geo-
 1057 metric uncertainty through adaptive experimental designs, active learning, derivative-information
 1058 selection, and more flexible polynomial truncation strategies. Additional developments may in-
 1059 corporate sensitivities with respect to multiple classes of uncertain parameters, including material
 1060 properties, and extend the formulation to more general constitutive models and large-scale engi-
 1061 neering applications.

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1068 Appendix A. Geometry-induced pseudo-load matrix in isogeometric analysis

1069 This appendix provides the explicit expressions of the geometry-induced pseudo-load matri-
 1070 ces introduced in Section 4.3. The first part summarizes the linear formulation, whereas the
 1071 second presents its nonlinear extension. Both derivations follow standard variational sensitivity
 1072 formulations for isogeometric analysis and are reported here for completeness.

1073 The global pseudo-load matrix $\mathbf{Q}(\mathbf{x})$ is assembled from elemental contributions as

$$\mathbf{Q}(\mathbf{x}) = \bigcup_{e=1}^{n_{\text{el}}} \mathbf{Q}_e(\mathbf{x}), \quad (\text{A.1})$$

1074 with

$$\mathbf{Q}_e(\mathbf{x}) = \int_{\Omega_e(\mathbf{x})} \sum_i \sum_j [\boldsymbol{\sigma}(\mathbf{x}) (\mathbf{L}_i(\mathbf{x}) \mathbf{L}_j^{\text{T}}(\mathbf{x}) - \mathbf{L}_j(\mathbf{x}) \mathbf{L}_i^{\text{T}}(\mathbf{x})) - \mathbf{B}_i^{\text{T}}(\mathbf{x}) \mathbf{C} \mathbf{B}_j(\mathbf{x}) \mathbf{H}(\mathbf{x})] \, \text{d}V. \quad (\text{A.2})$$

1075 Here, $\boldsymbol{\sigma}$ denotes the Cauchy stress tensor, $\mathbf{x}$ is the vector of uncertain geometric parameters, $\mathbf{B}_i$
 1076 the strain–displacement matrix associated with the i -th control-point, and $\mathbf{L}_i$ the matrix collecting
 1077 the spatial derivatives of the NURBS basis functions. n_{el} denotes the number of elements and n_{cp}^{e}

denotes the number of control points associated with element e . The matrix $\mathbf{H}(\mathbf{x})$ represents the element displacement gradient and is given by

$$\mathbf{H}(\mathbf{x}) = \nabla \mathbf{u}_e(\mathbf{x}) = \sum_{i=1}^{n_{\text{cp}}^e} \mathbf{u}_i(\mathbf{x}) \mathbf{L}_i^{\top}(\mathbf{x}). \quad (\text{A.3})$$

The above expressions follow standard variational sensitivity formulations for isogeometric analysis; see, e.g., [51, 14, 15].

The nonlinear pseudo-load matrix introduced in Eq. (45) is assembled element-wise within the Total-Lagrangian formulation adopted in this work. The resulting global pseudo-load matrix is given by

$$\mathbf{Q}_{\text{nl}}(\mathbf{x}) = \bigcup_{e=1}^{n_{\text{el}}} \mathbf{Q}_{\text{nl},e}(\mathbf{x}), \quad \mathbf{Q}_{\text{nl},e} = \mathbf{Q}_{\text{int,nl},e} - \mathbf{Q}_{\text{ext,nl},e}. \quad (\text{A.4})$$

Here, $\mathbf{Q}_{\text{int,nl},e}$ and $\mathbf{Q}_{\text{ext,nl},e}$ denote the geometric derivatives of the elemental internal- and external-force vectors, respectively. In the numerical examples considered in this work, body forces vanish and the prescribed external loads are independent of the uncertain geometry. Consequently, $\mathbf{Q}_{\text{ext,nl},e} = \mathbf{0}$.

For a two-dimensional element, the elemental internal pseudo-load matrix is expressed as

$$\mathbf{Q}_{\text{int,nl},e} = \int_{\Omega_{0,e}(\mathbf{x})} \left[\mathbf{B}_{\text{L},e}^{\top} \mathbf{C}_{\text{T}} \mathbf{B}_{\text{L},x,e} - (\mathbf{L}_e^{\top} \mathbf{S} \mathbf{L}_e) \otimes \nabla_{\mathbf{x}} \mathbf{u} - (\mathbf{I}_{n_{\text{cp}}^e} \otimes \mathbf{F} \mathbf{S}) \mathbf{L}_{\Delta,e} \right] dV_0. \quad (\text{A.5})$$

Here, $\Omega_{0,e}(\mathbf{x})$ denotes the elemental domain in the reference configuration and dV_0 is the corresponding differential volume element. The vector $\mathbf{X}$ denotes the material coordinates in the reference configuration, and $\mathbf{u}$ denotes the converged displacement field. The tensor $\mathbf{F}$ denotes the deformation gradient, $\mathbf{S}$ denotes the second Piola–Kirchhoff stress tensor, and $\mathbf{C}_{\text{T}}$ denotes the consistent material tangent matrix. The symbol $\otimes$ denotes the Kronecker product, and $\mathbf{I}_{n_{\text{cp}}^e}$ is the identity matrix of order n_{cp}^e . All geometric, kinematic, and constitutive quantities in Eq. (A.5) are evaluated at the converged equilibrium state and at the elemental quadrature points.

The elemental gradient and nonlinear strain–displacement operators are collected as

$$\mathbf{L}_e = \begin{bmatrix} \mathbf{L}_1 & \mathbf{L}_2 & \cdots & \mathbf{L}_{n_{\text{cp}}^e} \end{bmatrix}, \quad \mathbf{B}_{\text{L},e} = \begin{bmatrix} \mathbf{B}_{\text{L},1} & \mathbf{B}_{\text{L},2} & \cdots & \mathbf{B}_{\text{L},n_{\text{cp}}^e} \end{bmatrix}. \quad (\text{A.6})$$

1098 The corresponding explicit geometry-induced operator is defined as

$$\mathbf{B}_{L,x,e} = \begin{bmatrix} \mathbf{B}_{L,x,1} & \mathbf{B}_{L,x,2} & \cdots & \mathbf{B}_{L,x,n_{\text{cp}}^e} \end{bmatrix}, \quad \mathbf{B}_{L,x,e} = -\mathbf{B}_{L,e} (\mathbf{I}_{n_{\text{cp}}^e} \otimes \nabla_{\mathbf{x}} \mathbf{u}). \quad (\text{A.7})$$

1099 Using the deformation gradient defined in Eq. (28), the nonlinear strain–displacement operator
1100 associated with control-point i is

$$\mathbf{B}_{L,i} = \begin{bmatrix} F_{11}L_{i1} & F_{21}L_{i1} \\ F_{12}L_{i2} & F_{22}L_{i2} \\ F_{11}L_{i2} + F_{12}L_{i1} & F_{21}L_{i2} + F_{22}L_{i1} \end{bmatrix}. \quad (\text{A.8})$$

1101 The matrix $\mathbf{L}_{\Delta,e}$ collects the combinations of the elemental basis-function gradients appearing
1102 in the last term of Eq. (A.5). It is defined as

$$\mathbf{L}_{\Delta,e} = [\mathbf{L}_j \mathbf{L}_i^{\text{T}} - \mathbf{L}_i \mathbf{L}_j^{\text{T}}]_{i,j=1}^{n_{\text{cp}}^e}. \quad (\text{A.9})$$

1103 This definition provides a compact representation of the contributions $-\mathbf{F} \mathbf{S} \mathbf{L}_j \mathbf{L}_i^{\text{T}} + \mathbf{F} \mathbf{S} \mathbf{L}_i \mathbf{L}_j^{\text{T}}$ ap-
1104 pearing in the last term of Eq. (A.5).

1105 The Green–Lagrange strain and second Piola–Kirchhoff stress tensors are represented in vector
1106 form as

$$\mathbf{E}_v = \begin{bmatrix} E_{11} & E_{22} & 2E_{12} \end{bmatrix}^{\text{T}}, \quad \mathbf{S}_v = \begin{bmatrix} S_{11} & S_{22} & S_{12} \end{bmatrix}^{\text{T}}. \quad (\text{A.10})$$

1107 The consistent material tangent is defined by

$$\mathbf{C}_T = \frac{\partial \mathbf{S}_v}{\partial \mathbf{E}_v}, \quad (\text{A.11})$$

1108 where $\mathbf{S}$ is the second Piola–Kirchhoff stress tensor defined in Eq. (31).

1109 Finally, the elemental contributions are assembled into the global pseudo-load matrix $\mathbf{Q}_{\text{nl}}$.
1110 The resulting pseudo-load matrix is combined with the design-velocity matrix $\mathbf{D}$, which maps
1111 variations of the uncertain geometric parameters to variations of the control-point coordinates,
1112 according to Eq. (46). The resulting linear system yields the displacement sensitivities with respect
1113 to the uncertain geometric parameters. This formulation corresponds to the Total–Lagrangian
1114 specialization of the variational pseudo-load approach presented in [14, 15].

1115 Appendix B. Implementation details for the quarter-circular annulus

1116 The quarter-circular annulus is represented by a single NURBS surface with a 3×2 control
1117 net. The physical control-point matrix is given in Eq. (56). The NURBS weights are

$$\mathbf{W} = \begin{bmatrix} 1 & \frac{1}{\sqrt{2}} & 1 \\ 1 & \frac{1}{\sqrt{2}} & 1 \end{bmatrix}, \quad (\text{B.1})$$

1118 and the knot vectors are

$$\mathbf{\Xi} = [0, 0, 0, 1, 1, 1], \quad \mathbf{H} = [0, 0, 1, 1], \quad (\text{B.2})$$

1119 with polynomial degrees

$$(p, q) = (2, 1). \quad (\text{B.3})$$

1120 The design-velocity matrix maps variations of the uncertain parameters to variations of the
1121 physical control-point coordinates. For compactness, the transpose of the design-velocity matrix
1122 associated with Eq. (56) is reported as

$$\mathbf{D}^T = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix}, \quad (\text{B.4})$$

1123 where the first row contains the derivatives of the control-point coordinates with respect to the
1124 radius r , while the second row contains the derivatives with respect to the thickness t . Although the
1125 design-velocity matrix is constant for this affine parameterization, the total response sensitivities
1126 remain realization-dependent through the geometry-dependent stiffness matrix, geometry-induced
1127 pseudo-load terms, stress field, and response functional.

1128 Dirichlet boundary conditions are imposed at control points 1 and 4 in both displacement
1129 directions (see Figure 4), while nodal forces of 10 000 N are applied in the positive x -direction at
1130 control points 3 and 6. Body forces are set to zero.

1131 Appendix B.1. Illustrative stress-triaxiality distributions

1132 Figure B.15 shows the spatial stress-triaxiality distributions for selected geometric realizations
1133 of the quarter-circular annulus. The selected cases span nominal, near-boundary, and intermediate
1134 combinations of the uncertain radius r and thickness t . They illustrate the redistribution of the
1135 stress-triaxiality field induced by geometric variability.

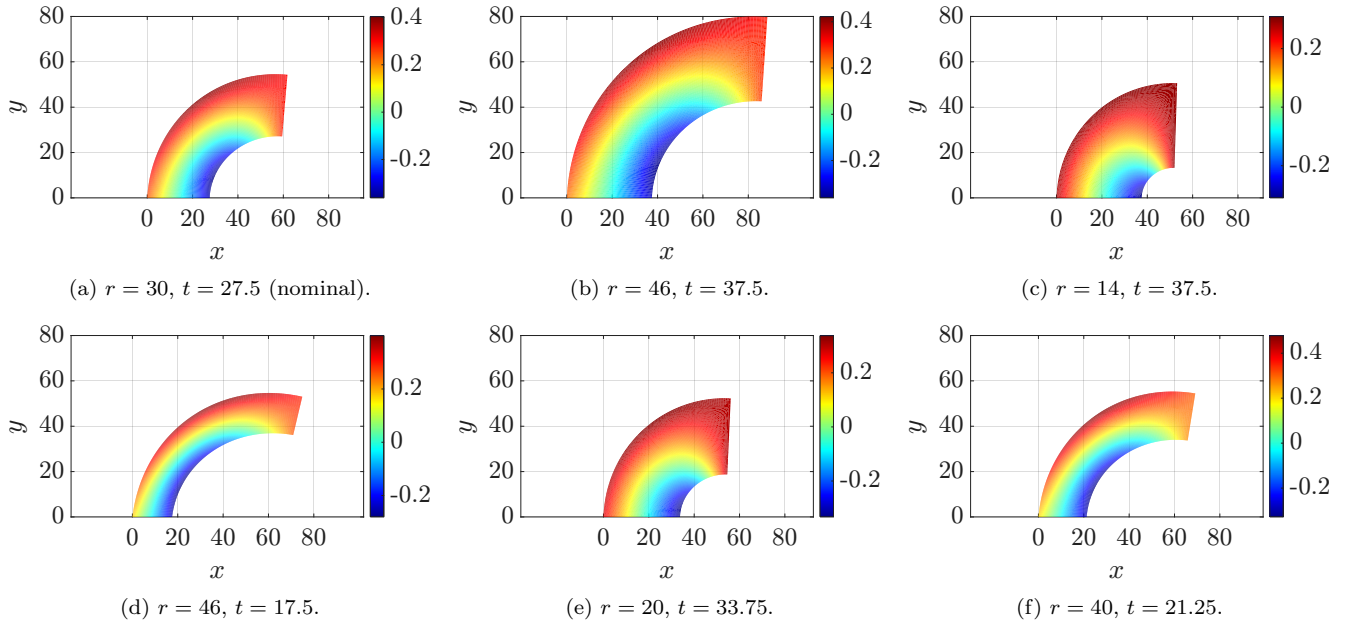


Figure B.15: Stress-triaxiality distributions for selected geometric realizations of the quarter-circular annulus over the deformed configuration. The cases span the admissible parameter ranges $r \in [10, 50]$ mm and $t \in [15, 40]$ mm and include nominal, near-boundary, and intermediate realizations. Independent color scales are intentionally used for each realization to emphasize geometry-induced spatial redistribution of stress triaxiality and the consistent physical location of the region of maximum stress triaxiality across the different geometries.

Appendix C. Gradient-enhanced Kriging benchmark

Gradient-enhanced Kriging (GEK–FD) was included as an external benchmark to compare the proposed IGA-based sensitivity-enhanced PCE formulation with a surrogate model from a different methodological family. Unless otherwise stated, the same implementation strategy was adopted throughout all numerical examples. Tables C.9 and C.10 summarize the principal implementation settings employed for each benchmark problem, including the covariance kernel, the gradient approximation strategy, the hyperparameter estimation procedure, the optimization strategy, and the statistical protocol adopted for the numerical experiments. Whenever required, example-specific modifications (e.g., multiple optimization starts for challenging nonlinear problems) are also reported. For every statistical repetition and training set, the GEK hyperparameters were re-estimated independently through maximum-likelihood optimization. This protocol avoids bias from previously calibrated models and ensures that the computational comparisons reported in the paper are performed under identical statistical conditions.

Table C.9: Core implementation settings of the GEK–FD benchmark used in the two-dimensional examples.

Setting	Specification
Inputs	(r, t) for the geometry-only examples and (r, t, ν) for the combined uncertainty example.
Kernel	Anisotropic squared exponential with one length scale per input variable.
Gradient data	Central finite differences with $h_r = h_t = 10^{-4}$; only the r and t derivatives are supplied in the combined uncertainty example.
Normalization	Inputs and responses are standardized using their training mean and standard deviation, with consistent scaling of the gradients.
Hyperparameters	Signal scale σ_f , one length scale ℓ_j per input, and separate response and gradient nuggets.
Estimation	Maximum likelihood using <code>fmincon</code> in logarithmic space with the interior-point algorithm and 10 multistarts comprising one reference and nine log-uniform initializations.
Search bounds	$\sigma_f \in [10^{-3}, 10^3]$, $\ell_j \in [0.05, 10]$, and nuggets in $[10^{-12}, 10^{-2}]$.

Table C.10: Core implementation settings of the GEK–FD benchmark for the three-dimensional horseshoe.

Setting	Specification
Inputs	(R, r, L, H) for the three-dimensional horseshoe.
Kernel	Anisotropic squared exponential with one length scale per input variable.
Gradient data	Central finite differences; all four geometric derivatives are supplied.
Normalization	Inputs and responses are standardized using their training mean and standard deviation, with consistent scaling of the gradients.
Hyperparameters	Signal scale σ_f , length scales $(\ell_R, \ell_r, \ell_L, \ell_H)$, and separate response and gradient nuggets.
Estimation	Maximum likelihood using <code>fmincon</code> in logarithmic space with the interior-point algorithm and 40 multistarts.
Search bounds	$\sigma_f \in [10^{-3}, 10^3]$, $(\ell_R, \ell_r, \ell_L, \ell_H) \in [0.1, 10] \times [0.1, 15] \times [0.3, 15] \times [1, 50]$, a response nugget in $[10^{-10}, 10^{-2}]$, and a gradient nugget in $[10^{-8}, 5 \times 10^{-2}]$.

1149 Appendix D. Parametric NURBS definition of the three-dimensional horseshoe

1150 The horseshoe geometry is represented by a NURBS volume with $4 \times 3 \times 9$ control points and
1151 quadratic basis functions in the three parametric directions. The control net depends explicitly
1152 on the uncertain geometric parameters (R, r, L, H) . The corresponding knot vectors and non-unit
1153 weights are shown in Table D.11.

1154 The NURBS volume is constructed from three cross-sectional curves, corresponding to the
1155 inner, middle, and outer curves of the horseshoe section, swept through nine stations. Each block
1156 $\mathbf{P}^{(b,c)} \in \mathbb{R}^{4 \times 4}$ contains four homogeneous control points as columns, where $b = 1, 2, 3$ denotes the

Table D.11: Knot vectors and NURBS weights used in the horseshoe geometry.

Quantity	Definition
Ξ	$[0, 0, 0, 1/2, 1, 1, 1]$
$\mathbf{H}$	$[0, 0, 0, 1, 1, 1]$
$\mathbf{Z}$	$[0, 0, 0, 1/6, 2/6, 1/2, 1/2, 4/6, 5/6, 1, 1, 1]$
w_1	$\frac{1}{2} \left(1 + \frac{1}{\sqrt{2}} \right)$
w_2	$\frac{1}{\sqrt{2}}$
w_3	$w_1 w_2$

1157 curve index and $c = 1, \dots, 9$ denotes the sweep station. The rows of each block correspond to
 1158 weighted coordinates (xw, yw, zw, w) . Physical coordinates are obtained by dehomogenization.

1159 The following tables report the homogeneous control-point matrices defining the complete
 1160 parametric NURBS volume. The design-velocity matrix $\mathbf{D} \in \mathbb{R}^{324 \times 4}$ used in the sensitivity analysis
 1161 can be obtained by analytically differentiating the physical control-point coordinates with respect
 1162 to (R, r, L, H) .

1163 *Appendix D.1. Illustrative stress-triaxiality distributions*

1164 Figure D.16 shows the stress-triaxiality distributions for selected geometric realizations of the
 1165 three-dimensional horseshoe-shaped solid. The three-dimensional and in-plane views illustrate the
 1166 geometry-induced redistribution of the stress field over the deformed configurations. Independent
 1167 color scales are used to emphasize variations in the spatial distribution of stress triaxiality.

Table D.12: Parametric control-point matrices for the horseshoe NURBS volume: left straight side.

Station	Curve	Control-point matrix $\mathbf{P}^{(b,c)}$
$c = 1$	Inner	$\begin{bmatrix} -R & -Rw_1 & -\frac{R}{2}w_1 & 0 \\ 0 & \frac{R}{2}w_1 & Rw_1 & R \\ 0 & 0 & 0 & 0 \\ 1 & w_1 & w_1 & 1 \end{bmatrix}$
	Middle	$\begin{bmatrix} -\left(\frac{L-R}{2} + R\right) & -\left(\frac{L-R}{2} + R\right) & -R & 0 \\ 0 & R & \left(\frac{L-R}{2} + R\right) & \left(\frac{L-R}{2} + R\right) \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$
	Outer	$\begin{bmatrix} -L & -L & -\frac{7}{8}L & 0 \\ 0 & \frac{7}{8}L & L & L \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$
$c = 2$	Inner	$\begin{bmatrix} -R & -Rw_1 & -\frac{R}{2}w_1 & 0 \\ 0 & \frac{R}{2}w_1 & Rw_1 & R \\ \frac{H}{4} & \frac{H}{4}w_1 & \frac{H}{4}w_1 & \frac{H}{4} \\ 1 & w_1 & w_1 & 1 \end{bmatrix}$
	Middle	$\begin{bmatrix} -\left(\frac{L-R}{2} + R\right) & -\left(\frac{L-R}{2} + R\right) & -R & 0 \\ 0 & R & \left(\frac{L-R}{2} + R\right) & \left(\frac{L-R}{2} + R\right) \\ \frac{H}{4} & \frac{H}{4} & \frac{H}{4} & \frac{H}{4} \\ 1 & 1 & 1 & 1 \end{bmatrix}$
	Outer	$\begin{bmatrix} -L & -L & -\frac{7}{8}L & 0 \\ 0 & \frac{7}{8}L & L & L \\ \frac{H}{4} & \frac{H}{4} & \frac{H}{4} & \frac{H}{4} \\ 1 & 1 & 1 & 1 \end{bmatrix}$
$c = 3$	Inner	$\begin{bmatrix} -R & -Rw_1 & -\frac{R}{2}w_1 & 0 \\ 0 & \frac{R}{2}w_1 & Rw_1 & R \\ \frac{H}{2} & \frac{H}{2}w_1 & \frac{H}{2}w_1 & \frac{H}{2} \\ 1 & w_1 & w_1 & 1 \end{bmatrix}$
	Middle	$\begin{bmatrix} -\left(\frac{L-R}{2} + R\right) & -\left(\frac{L-R}{2} + R\right) & -R & 0 \\ 0 & R & \left(\frac{L-R}{2} + R\right) & \left(\frac{L-R}{2} + R\right) \\ \frac{H}{2} & \frac{H}{2} & \frac{H}{2} & \frac{H}{2} \\ 1 & 1 & 1 & 1 \end{bmatrix}$
	Outer	$\begin{bmatrix} -L & -L & -\frac{7}{8}L & 0 \\ 0 & \frac{7}{8}L & L & L \\ \frac{H}{2} & \frac{H}{2} & \frac{H}{2} & \frac{H}{2} \\ 1 & 1 & 1 & 1 \end{bmatrix}$

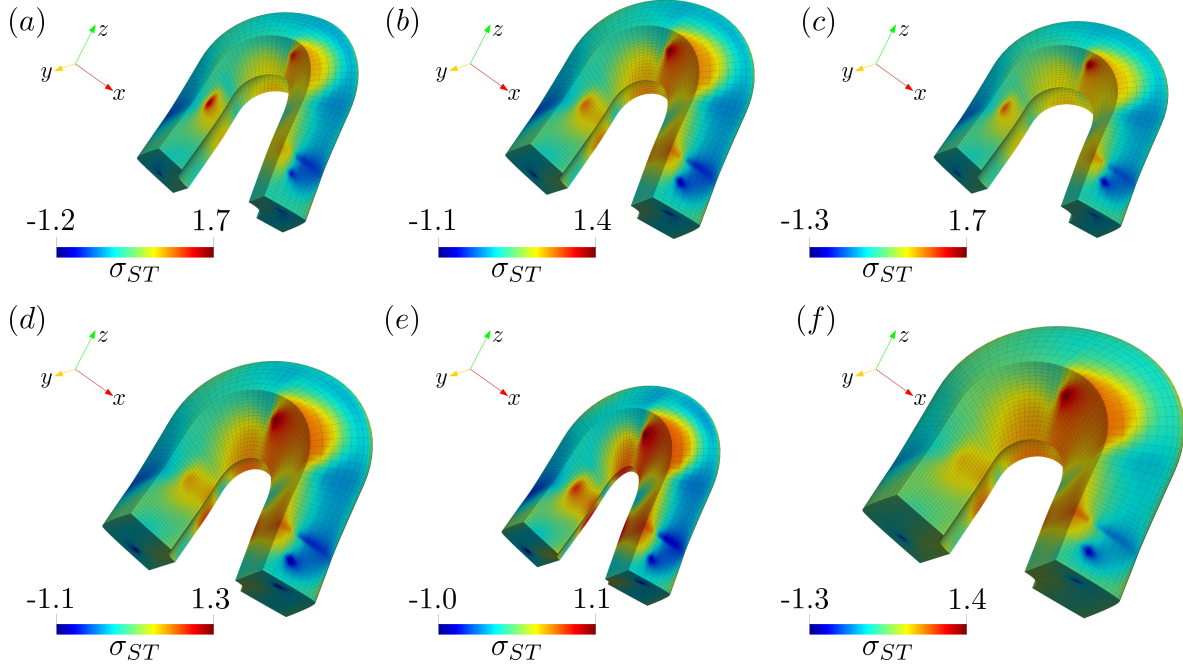
Table D.13: Parametric control-point matrices for the horseshoe NURBS volume: transition and top sections.

Station	Curve	Control-point matrix $\mathbf{P}^{(b,c)}$
$c = 4$	Inner	$\begin{bmatrix} -Rw_2 & -Rw_3 & -\frac{R}{2}w_3 & 0 \\ 0 & \frac{R}{2}w_3 & Rw_3 & Rw_2 \\ Hw_2 & (H + Rw_2)w_3 & (H + Rw_2)w_3 & Hw_2 \\ w_2 & w_3 & w_3 & w_2 \end{bmatrix}$
$c = 4$	Middle	$\begin{bmatrix} -\left(\frac{L-R}{2} + R\right)w_2 & -\left(\frac{L-R}{2} + R\right)w_2 & -Rw_2 & 0 \\ 0 & Rw_2 & \left(\frac{L-R}{2} + R\right)w_2 & \left(\frac{L-R}{2} + R\right)w_2 \\ \left(H + L - R - \frac{L-R}{2}w_2\right)w_2 & \left(H + L - \frac{L-R}{2}w_2\right)w_2 & \left(H + L - \frac{L-R}{2}w_2\right)w_2 & \left(H + L - R - \frac{L-R}{2}w_2\right)w_2 \\ w_2 & w_2 & w_2 & w_2 \end{bmatrix}$
$c = 4$	Outer	$\begin{bmatrix} -Lw_2 & -Lw_2 & -\frac{7}{8}Lw_2 & 0 \\ 0 & \frac{7}{8}Lw_2 & Lw_2 & Lw_2 \\ (H + L - R)w_2 & \left(H + L - R + \frac{7}{8}L\right)w_2 & \left(H + L - R + \frac{7}{8}L\right)w_2 & (H + L - R)w_2 \\ w_2 & w_2 & w_2 & w_2 \end{bmatrix}$
$c = 5$	Inner	$\begin{bmatrix} 0 & \frac{R}{4}w_1 & \frac{3R}{4}w_1 & R \\ -R & -\frac{3R}{4}w_1 & -\frac{R}{4}w_1 & 0 \\ H & (H + Rw_2)w_1 & (H + Rw_2)w_1 & H \\ 1 & w_1 & w_1 & 1 \end{bmatrix}$
$c = 5$	Middle	$\begin{bmatrix} -\frac{L-R}{4} & \frac{3R-L}{4} & \frac{R+L}{4} & \frac{L+3R}{4} \\ -\frac{L+3R}{4} & -\frac{R+L}{4} & -\frac{3R-L}{4} & \frac{L-R}{4} \\ H + L - R - \frac{L-R}{2}w_2 & H + L - \frac{L-R}{2}w_2 & H + L - \frac{L-R}{2}w_2 & H + L - R - \frac{L-R}{2}w_2 \\ 1 & 1 & 1 & 1 \end{bmatrix}$
$c = 5$	Outer	$\begin{bmatrix} \frac{R-L}{2} & \frac{R}{4} & \frac{3R}{4} & \frac{R+L}{2} \\ -\frac{R+L}{2} & -\frac{3R}{4} & -\frac{R}{4} & -\frac{R-L}{2} \\ H + L - R & H + L - R + \frac{7}{8}L & H + L - R + \frac{7}{8}L & H + L - R \\ 1 & 1 & 1 & 1 \end{bmatrix}$
$c = 6$	Inner	$\begin{bmatrix} rw_2^2 & (rw_2 + \frac{R}{2})w_3 & (rw_2 + R)w_3 & (rw_2 + R)w_2 \\ -(rw_2 + R)w_2 & -(rw_2 + R)w_3 & -(rw_2 + \frac{R}{2})w_3 & -rw_2^2 \\ Hw_2 & (H + Rw_2)w_3 & (H + Rw_2)w_3 & Hw_2 \\ w_2 & w_3 & w_3 & w_2 \end{bmatrix}$
$c = 6$	Middle	$\begin{bmatrix} rw_2^2 & (rw_2 + R)w_2 & \left(rw_2 + \frac{L-R}{2} + R\right)w_2 & \left(rw_2 + \frac{L-R}{2} + R\right)w_2 \\ -\left(rw_2 + \frac{L-R}{2} + R\right)w_2 & -\left(rw_2 + \frac{L-R}{2} + R\right)w_2 & -(rw_2 + R)w_2 & -rw_2^2 \\ \left(H + L - R - \frac{L-R}{2}w_2\right)w_2 & \left(H + L - \frac{L-R}{2}w_2\right)w_2 & \left(H + L - \frac{L-R}{2}w_2\right)w_2 & \left(H + L - R - \frac{L-R}{2}w_2\right)w_2 \\ w_2 & w_2 & w_2 & w_2 \end{bmatrix}$
$c = 6$	Outer	$\begin{bmatrix} rw_2^2 & \left(\frac{7}{8}L + rw_2\right)w_2 & (rw_2 + L)w_2 & (rw_2 + L)w_2 \\ -(rw_2 + L)w_2 & -(rw_2 + L)w_2 & -\left(\frac{7}{8}L + rw_2\right)w_2 & -rw_2^2 \\ (H + L - R)w_2 & \left(H + L - R + \frac{7}{8}L\right)w_2 & \left(H + L - R + \frac{7}{8}L\right)w_2 & (H + L - R)w_2 \\ w_2 & w_2 & w_2 & w_2 \end{bmatrix}$

Table D.14: Parametric control-point matrices for the horseshoe NURBS volume: right straight side.

Station	Curve	Control-point matrix $\mathbf{P}^{(b,c)}$
$c = 7$	Inner	$\begin{bmatrix} rw_2 & \left(rw_2 + \frac{R}{2}\right)w_1 & (rw_2 + R)w_1 & rw_2 + R \\ -(rw_2 + R) & -(rw_2 + R)w_1 & -\left(rw_2 + \frac{R}{2}\right)w_1 & -rw_2 \\ \frac{H}{2} & \frac{H}{2}w_1 & \frac{H}{2}w_1 & \frac{H}{2} \\ 1 & w_1 & w_1 & 1 \end{bmatrix}$
$c = 7$	Middle	$\begin{bmatrix} rw_2 & rw_2 + R & rw_2 + \frac{L-R}{2} + R & rw_2 + \frac{L-R}{2} + R \\ -\left(rw_2 + \frac{L-R}{2} + R\right) & -\left(rw_2 + \frac{L-R}{2} + R\right) & -(rw_2 + R) & -rw_2 \\ \frac{H}{2} & \frac{H}{2} & \frac{H}{2} & \frac{H}{2} \\ 1 & 1 & 1 & 1 \end{bmatrix}$
$c = 7$	Outer	$\begin{bmatrix} rw_2 & \frac{7}{8}L + rw_2 & rw_2 + L & rw_2 + L \\ -(rw_2 + L) & -(rw_2 + L) & -\left(\frac{7}{8}L + rw_2\right) & -rw_2 \\ \frac{H}{2} & \frac{H}{2} & \frac{H}{2} & \frac{H}{2} \\ 1 & 1 & 1 & 1 \end{bmatrix}$
$c = 8$	Inner	$\begin{bmatrix} rw_2 & \left(rw_2 + \frac{R}{2}\right)w_1 & (rw_2 + R)w_1 & rw_2 + R \\ -(rw_2 + R) & -(rw_2 + R)w_1 & -\left(rw_2 + \frac{R}{2}\right)w_1 & -rw_2 \\ \frac{H}{4} & \frac{H}{4}w_1 & \frac{H}{4}w_1 & \frac{H}{4} \\ 1 & w_1 & w_1 & 1 \end{bmatrix}$
$c = 8$	Middle	$\begin{bmatrix} rw_2 & rw_2 + R & rw_2 + \frac{L-R}{2} + R & rw_2 + \frac{L-R}{2} + R \\ -\left(rw_2 + \frac{L-R}{2} + R\right) & -\left(rw_2 + \frac{L-R}{2} + R\right) & -(rw_2 + R) & -rw_2 \\ \frac{H}{4} & \frac{H}{4} & \frac{H}{4} & \frac{H}{4} \\ 1 & 1 & 1 & 1 \end{bmatrix}$
$c = 8$	Outer	$\begin{bmatrix} rw_2 & \frac{7}{8}L + rw_2 & rw_2 + L & rw_2 + L \\ -(rw_2 + L) & -(rw_2 + L) & -\left(\frac{7}{8}L + rw_2\right) & -rw_2 \\ \frac{H}{4} & \frac{H}{4} & \frac{H}{4} & \frac{H}{4} \\ 1 & 1 & 1 & 1 \end{bmatrix}$
$c = 9$	Inner	$\begin{bmatrix} rw_2 & \left(rw_2 + \frac{R}{2}\right)w_1 & (rw_2 + R)w_1 & rw_2 + R \\ -(rw_2 + R) & -(rw_2 + R)w_1 & -\left(rw_2 + \frac{R}{2}\right)w_1 & -rw_2 \\ 0 & 0 & 0 & 0 \\ 1 & w_1 & w_1 & 1 \end{bmatrix}$
$c = 9$	Middle	$\begin{bmatrix} rw_2 & rw_2 + R & rw_2 + \frac{L-R}{2} + R & rw_2 + \frac{L-R}{2} + R \\ -\left(rw_2 + \frac{L-R}{2} + R\right) & -\left(rw_2 + \frac{L-R}{2} + R\right) & -(rw_2 + R) & -rw_2 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$
$c = 9$	Outer	$\begin{bmatrix} rw_2 & \frac{7}{8}L + rw_2 & rw_2 + L & rw_2 + L \\ -(rw_2 + L) & -(rw_2 + L) & -\left(\frac{7}{8}L + rw_2\right) & -rw_2 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$

Three-dimensional view



In-plane view

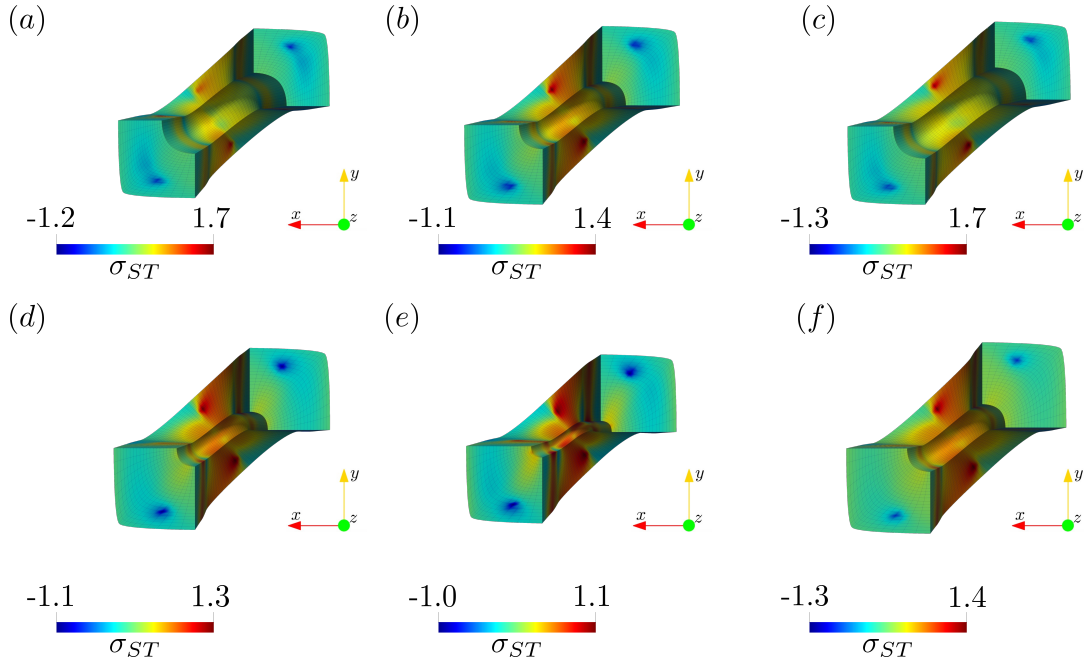


Figure D.16: Stress triaxiality distributions for selected geometric realizations of the three-dimensional horseshoe-shaped solid. The upper panel shows a three-dimensional view of the deformed configurations, while the lower panel shows the corresponding in-plane view. The six cases correspond to: (a) $R = 1.5$, $r = \sqrt{2} - 0.5$, $L = 3.5$, $H = 8.5$; (b) $R = 1.2$, $r = \sqrt{2}$, $L = 4.0$, $H = 8.2$; (c) $R = 1.5$, $r = 1.7978$, $L = 3.6652$, $H = 7.5$; (d) $R = 1.0$, $r = \sqrt{2}$, $L = 4.5$, $H = 8.0$; (e) $R = 0.5$, $r = \sqrt{2} - 0.5$, $L = 3.5$, $H = 7.5$; and (f) $R = 1.5$, $r = \sqrt{2} + 0.5$, $L = 5.5$, $H = 8.5$. Independent color scales are used to emphasize geometry-induced spatial redistribution of stress triaxiality. All dimensions are given in cm.

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